Catalyst-Free Four-Component Domino Reaction for Synthesis of Functionalized 3-Acyl-1,5-Benzodiazepines

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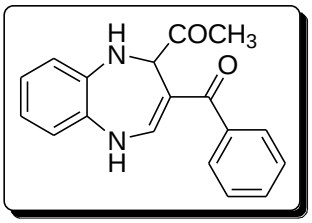
Content **Page Numbers**

3-acyl-1,5-benzodiazepine 5aaa



Yield: 84%;

Characteristic: Yellow solid;

M.P.: 188-189 ℃;

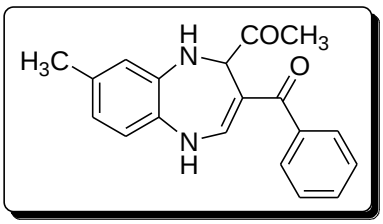
IR (KBr): 3330, 1704, 1635, 1540 cm^{-1};

^{1}H NMR (400 MHz, DMSO-d_6, TMS): δ 2.14 (3H, s, Me), 5.24 (1H, d, *J*=4.0 Hz, CH), 6.52 (1H, d, *J*=4.0 Hz, NH), 6.71-6.88 (4H, m, Ph), 7.10 (1H, d, *J*=6.4 Hz, CH), 7.46 (5H, s, Ph), 9.52 (1H, d, *J*=6.4 Hz, NH);

^{13}C NMR (100 MHz, DMSO-d_6, TMS): δ 28.7, 63.0, 120.3, 120.6, 120.9, 123.9, 128.6, 130.2, 138.5, 140.7, 146.7, 192.9, 205.8;

Found C, 73.87; H, 5.36; N, 9.74%; M+1 (mass spectrum), 293.2. $C_{18}H_{16}N_2O_2$ requires C, 73.95; H, 5.52; N, 9.58%; M, 292.34.

3-acyl-1,5-benzodiazepine 5aba



Yield: 89%;

Characteristic: Pale yellow solid;

M.P.: 168-170 ℃;

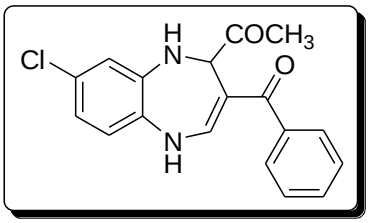
IR (KBr): 3334, 1702, 1635,1538 cm^{-1};

^{1}H NMR (400 MHz, DMSO-d_6, TMS): δ 2.14 (3H, s, Me), 2.17 (3H, s, Me), 5.22 (1H, d, *J*=2.4 Hz, CH), 6.44 (1H, d, *J*=2.4 Hz, NH), 6.53-6.70 (3H, m, Ph), 7.08 (1H, d, *J*=5.6 Hz, CH), 7.46 (5H, s, Ph), 9.48 (1H, d, *J*=6.0 Hz, NH);

^{13}C NMR (100 MHz, DMSO-d$_6$, TMS): δ 20.8, 28.7, 62.8, 110.1, 120.5, 121.1, 127.7, 128.6, 130.1, 132.9, 138.3, 140.8, 146.6, 192.6, 205.8;

Found C, 74.38; H, 5.69; N, 9.22%; M+1 (mass spectrum), 307.2. $C_{19}H_{18}N_2O_2$ requires C, 74.49; H, 5.92; N, 9.14%; M, 306.37.

3-acyl-1,5-benzodiazepine 5aca



Yield: 81%;

Characteristic: Yellow solid;

M.P.: 186-188 ℃;

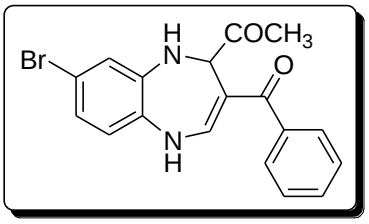
IR (KBr): 3340, 1702, 1635, 1527 cm^{-1};

^{1}H NMR (400 MHz, DMSO-d$_6$, TMS): δ 2.16 (3H, s, Me), 5.29 (1H, d, *J*=5.6 Hz, CH), 6.69 (1H, d, *J*=5.6 Hz, NH), 6.73-6.92 (3H, m, Ph), 7.09 (1H, d, *J*=8.0 Hz, CH), 7.47 (5H, s, Ph), 9.64 (1H, d, *J*=8.0 Hz, NH);

^{13}C NMR (100 MHz, DMSO-d$_6$, TMS): δ 28.8, 62.6, 110.5, 119.5, 119.6, 121.8, 127.2, 128.5, 128.6, 128.9, 130.3, 140.0, 140.5, 146.2, 192.9, 205.6;

Found C, 66.24; H, 4.79; N, 8.46%; M+1 (mass spectrum), 327.2. $C_{18}H_{15}ClN_2O_2$ requires C, 66.16; H, 4.63; N, 8.57%; M, 326.78.

3-acyl-1,5-benzodiazepine 5ada



Yield: 79%;

Characteristic: Light yellow solid;

M.P.: 181-183 ℃;

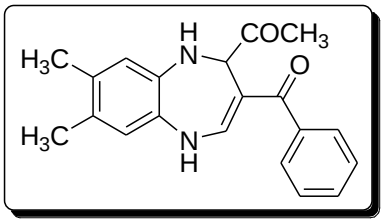
IR (KBr): 3337, 1700, 1644, 1528 cm^{-1};

^{1}H NMR (400 MHz, DMSO-d_6, TMS): δ 2.19 (3H, s, Me), 5.31 (1H, d, *J*=5.6 Hz, CH), 6.76 (1H, d, *J*=5.6 Hz, NH), 6.81-7.13 (3H, m, Ph), 7.09 (1H, d, *J*=7.6 Hz, CH), 7.50 (5H, s, Ph), 9.85 (1H, d, *J*=6.4 Hz, NH);

^{13}C NMR (100 MHz, DMSO-d_6, TMS): δ 28.8, 62.5, 110.4, 115.1, 122.2, 122.2, 122.4, 128.5, 128.6, 129.4, 130.3, 140.4, 140.5, 146.2, 192.8, 205.7;

Found C, 58.31; H, 4.21; N, 7.41%; M+1 (mass spectrum), 372.2. $C_{18}H_{15}BrN_2O_2$ requires C, 58.24; H, 4.07; N, 7.55%; M, 371.23.

3-acyl-1,5-benzodiazepine 5aea



Yield: 93%;

Characteristic: Deep yellow solid;

M.P.: 179-180 ℃;

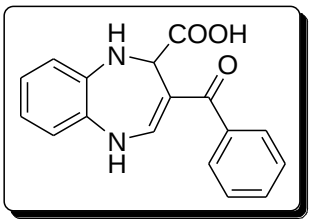
IR (KBr): 3334, 1696, 1635, 1527 cm^{-1};

^{1}H NMR 400 MHz, DMSO-d_6, TMS): δ 2.05 (3H, s, Me), 2.08 (3H, s, Me), 2.12 (3H, s, Me), 5.18 (1H, d, *J*=5.6 Hz, CH), 6.31 (1H, d, *J*=5.6 Hz, NH), 6.55-6.63 (2H, m, Ph), 7.06 (1H, d, *J*=8.0 Hz, CH), 7.45 (5H, s, Ph), 9.38 (1H, d, *J*=8.0 Hz, NH);

^{13}C NMR (100 MHz, DMSO-d_6, TMS): δ 18.8, 19.2, 28.7, 63.0, 110.3, 121.4, 121.8, 127.8, 127.9, 128.5, 128.6, 130.0, 131.7, 135.9, 140.9, 146.7, 192.6, 205.8;

Found C, 74.89; H, 6.11; N, 8.88%; M+1 (mass spectrum), 321.2. $C_{20}H_{20}N_2O_2$ requires C, 74.98; H, 6.29; N, 8.74%; M, 320.3.

3-acyl-1,5-benzodiazepine 5aab



Yield: 91%;

Characteristic: Yellow solid;

M.P.: 177-179 ℃;

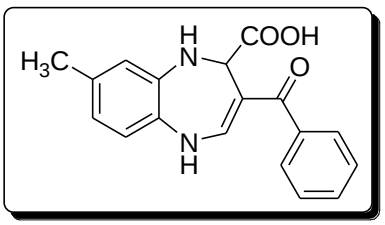
IR (KBr): 3333, 1684, 1639, 1534 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 5.15 (1H, d, *J*=5.0 Hz, CH), 6.32 (1H, d, *J*=5.0 Hz, NH), 6.73-6.89(4H, m, Ph), 7.05 (1H, d, *J*=8.5 Hz, CH), 7.45-7.48 (5H, m, Ph), 9.47 (1H, d, *J*=8.0 Hz, NH), 12.23 (1H, s, COOH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 57.7, 111.4, 120.4, 120.6, 121.5, 123.7, 128.5, 128.6, 130.2,130.7, 138.9, 140.8, 146.6, 172.9, 192.7;

Found C, 69.41; H, 4.74; N, 9.49%; M+1 (mass spectrum), 295.2. $C_{17}H_{14}N_2O_3$ requires C, 69.38; H, 4.79; N, 9.52%; M, 294.31.

3-acyl-1,5-benzodiazepine 5abb



Yield: 94%;

Characteristic: Pale yellow solid;

M.P.: 189-190 ℃;

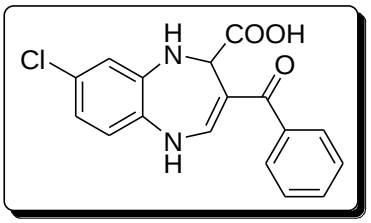
IR (KBr): 3325, 1717, 1637, 1518 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 2.17 (3H, s, Me), 5.16 (1H, d, *J*=4.0 Hz, CH), 6.25 (1H, d, *J*=4.5 Hz, NH), 6.56-6.72 (3H, m, Ph), 7.05 (1H, d, *J*=8.5 Hz, CH), 7.45-7.48 (5H, m, Ph), 9.43 (1H, d, *J*=8.5 Hz, NH), 12.22 (1H, s, COOH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 20.8, 57.6, 111.0, 120.4, 121.4, 121.7, 128.3, 128.5, 128.6, 130.1, 132.7, 138.7, 140.9, 146.6, 172.9, 192.5;

Found C, 70.26; H, 5.32; N, 8.89%; M+1 (mass spectrum), 309.2. $C_{18}H_{16}N_2O_3$ requires C, 70.12; H, 5.23; N, 9.09%; M, 308.34.

3-acyl-1,5-benzodiazepine 5acb



Yield: 89%;

Characteristic: Purple solid;

M.P.: 204-206 ℃;

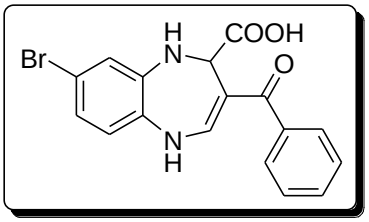
IR (KBr): 3318, 1709, 1645, 1534 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 5.16 (1H, d, J=5.5 Hz, CH), 6.60 (1H, d, J=5.5 Hz, NH), 6.77-6.93 (3H, m, Ph), 7.03 (1H, d, J=8.0 Hz, CH), 7.45-7.49 (5H, m, Ph), 9.57 (1H, d, J=8.0 Hz, NH), 12.36 (1H, s, COOH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 57.4, 111.5, 120.0, 120.3, 121.7, 127.0, 128.6, 128.6, 129.7, 130.3, 140.3, 140.6, 146.0, 172.7, 192.7;

Found C, 62.25; H, 4.11; N, 8.39%; M+1 (mass spectrum), 329.2. $C_{17}H_{13}ClN_2O_3$ requires C, 62.11; H, 3.99; N, 8.52%; M, 328.75.

3-acyl-1,5-benzodiazepine 5adb



Yield: 88%;

Characteristic: Yellow solid;

M.P.: 200-202 ℃;

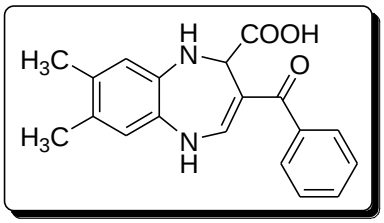
IR (KBr): 3302, 1725, 1645, 1549 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 5.17 (1H, d, *J*=5.5 Hz, CH), 6.60 (1H, d, *J*=5.5 Hz, NH), 6.76-7.06 (3H, m, Ph), 7.08 (1H, d, *J*=8.0 Hz, CH), 7.45-7.50 (5H, m, Ph), 9.57 (1H, d, *J*=8.0 Hz, NH), 12.38 (1H, s, COOH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 57.5, 111.6, 115.0, 122.0, 122.9, 123.2, 128.6, 128.6, 130.1, 130.3, 140.5, 140.6, 146.0, 172.6, 192.7;

Found C, 54.66; H, 3.39; N, 7.65%; M+1 (mass spectrum), 373.1. $C_{17}H_{13}BrN_2O_3$ requires C, 54.71; H, 3.51; N, 7.51%; M, 372.21.

3-acyl-1,5-benzodiazepine 5aeb



Yield: 95%;

Characteristic: Yellow solid;

M.P.: 191-193 ℃;

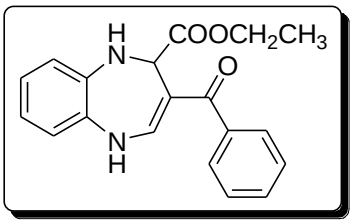
IR (KBr): 3357, 1749, 1621, 1502 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 2.06 (3H, s, Me), 2.08 (3H, s, Me), 5.11 (1H, d, *J*=5.0 Hz, CH), 6.05 (1H, d, *J*=5.5 Hz, NH), 6.57-6.65 (2H, m, Ph), 7.02 (1H, d, *J*=8.5 Hz, CH), 7.42-7.48 (5H, m, Ph), 9.32 (1H, d, *J*=8.5 Hz, NH), 12.12 (1H, s, COOH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 18.9, 19.2, 57.8, 111.1, 121.3, 122.6, 128.2, 128.3, 128.5, 128.6, 130.0, 131.5, 136.5, 141.0, 146.7, 172.9, 192.6;

Found C, 70.68; H, 5.49; N, 8.73%; M+1 (mass spectrum), 323.3. $C_{19}H_{18}N_2O_3$ requires C, 70.79; H, 5.63; N, 8.69%; M, 322.36.

3-acyl-1,5-benzodiazepine 5aac



Yield: 86%;

Characteristic: Pale yellow solid;

M.P.: 90-92 ℃;

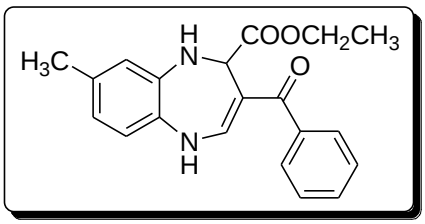
IR (KBr): 3333, 1709, 1637, 1526 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 0.98 (3H, t, *J*=7.0, Me), 3.93 (2H, q, *J*=6.5, CH_2), 5.22 (1H, d, *J*=5.5 Hz, CH), 6.43 (1H, d, *J*=5.5 Hz, NH), 6.76-6.89 (4H, m, Ph), 7.09 (1H, d, *J*=8.0 Hz, CH), 7.46-7.46 (5H, m, Ph), 9.51 (1H, d, *J*=8.0 Hz, NH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 14.6, 57.7, 60.6, 110.8, 120.4, 120.9, 121.5, 123.8, 128.5, 128.6, 130.2, 131.0, 138.5, 140.7, 146.7, 171.3, 192.5;

Found C, 70.83; H, 5.69; N, 8.61%; M+1 (mass spectrum), 323.2. $C_{19}H_{18}N_2O_3$ requires C, 70.79; H, 5.63; N, 8.69%; M, 322.36.

3-acyl-1,5-benzodiazepine 5abc



Yield: 90%;

Characteristic: Pale yellow solid;

M.P.: 94-96 ℃;

IR (KBr): 3333, 1717, 1637, 1541 cm^{-1};

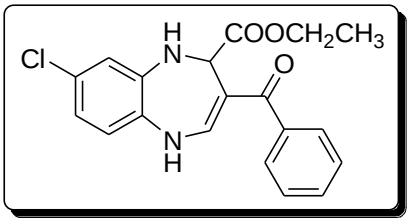
^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 1.00 (3H, t, *J*=6.0, Me), 2.17 (3H, s, Me), 3.94 (2H, q, *J*=6.0, CH_2), 5.21 (1H, d, *J*=5.5 Hz, CH), 6.33 (1H, d, *J*=6.0

Hz, NH), 6.58-6.74 (3H, m, Ph), 7.07 (1H, d, *J*=8.0 Hz, CH), 7.45-7.49 (5H, m, Ph), 9.46 (1H, d, *J*=8.0 Hz, NH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ14.6, 20.8, 57.6, 60.5, 110.5, 120.4, 121.6, 121.7, 128.4, 128.5, 128.6, 130.1, 132.8, 138.3, 140.9, 146.6, 171.4, 192.3;

Found C, 71.53; H, 6.11; N, 8.17%; M+1 (mass spectrum), 337.2. $C_{20}H_{20}N_2O_3$ requires C, 71.41; H, 5.99; N, 8.33%; M, 336.39.

3-acyl-1,5-benzodiazepine 5acc



Yield: 77%;

Characteristic: Purple solid;

M.P.: 100-102 ℃;

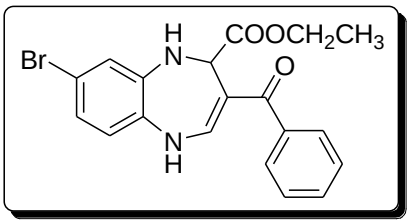
IR (KBr): 3322, 1715, 1640, 1549 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 1.03 (3H, t, *J*=6.5, Me), 3.99 (2H, q, *J*=6.5, CH_2), 5.24 (1H, d, *J*=5.0 Hz, CH), 6.69 (1H, d, *J*=4.5 Hz, NH), 6.79-7.09 (3H, m, Ph), 6.95 (1H, d, *J*=8.0 Hz, CH), 7.47 (5H, m, Ph), 9.62 (1H, d, *J*=7.5 Hz, NH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 14.6, 57.4, 60.8, 110.9, 120.3, 120.4, 121.7, 127.1, 128.5, 128.6, 129.9, 130.3, 139.9, 140.5, 146.1, 171.1,192.5;

Found C, 63.82; H, 4.67; N, 7.99%; M+1 (mass spectrum), 357.2. $C_{19}H_{17}ClN_2O_3$ requires C, 63.96; H, 4.80; N 7.85%; M, 356.81.

3-acyl-1,5-benzodiazepine 5adc



Yield: 82%;

Characteristic: Yellow solid;

M.P.: 102-104 ℃;

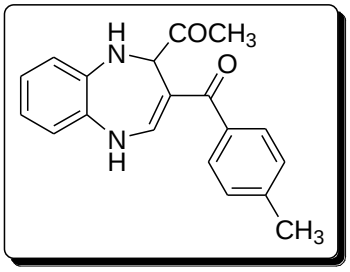
IR (KBr): 3286, 1716, 1637, 1549 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 0.97 (3H, t, *J*=6.5, Me), 3.93 (2H, q, *J*=6.5, CH_2), 5.18 (1H, d, *J*=5.0 Hz, CH), 6.63 (1H, d, *J*=4.5 Hz, NH), 6.79-7.03 (3H, m, Ph), 6.89 (1H, d, *J*=8.0 Hz, CH), 7.41 (5H, m, Ph), 9.56 (1H, d, *J*=7.0 Hz, NH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 14.6, 57.4, 60.8, 111.0, 115.1, 122.0, 123.2, 123.3, 128.5, 128.6, 130.3, 130.3, 140.2, 140.5, 146.1, 171.1, 192.5;

Found C, 56.76; H, 4.12; N, 7.11%; M+1 (mass spectrum), 403.1. $C_{19}H_{17}BrN_2O_3$ requires C, 56.87; H, 4.27; N, 6.98%; M, 402.04.

3-acyl-1,5-benzodiazepine 5baa



Yield: 88%;

Characteristic: Pale yellow solid;

M.P.: 193-194 ℃;

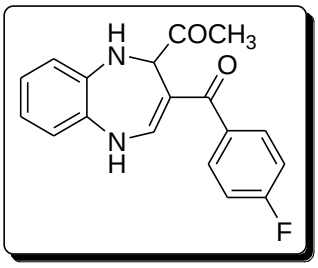
IR (KBr): 3334, 1702, 1635, 1533 cm^{-1};

^{1}H NMR (400 MHz, DMSO-d_6, TMS): δ 2.14 (3H, s, Me), 2.36 (3H, s, Me), 5.22 (1H, d, *J*=5.6 Hz, CH), 6.49 (1H, d, *J*=5.6 Hz, NH), 6.70-6.87 (4H, m, Ph), 7.11 (1H, d, *J*=8.0 Hz, CH), 7.25-7.38 (4H, m, Ph), 9.45 (1H, d, *J*=8.0 Hz, NH);

^{13}C NMR (100 MHz, DMSO-d_6, TMS): δ 21.4, 28.7, 63.1, 110.6, 120.3, 120.8, 123.8, 128.7, 129.1, 130.2, 137.8, 138.4, 139.9, 146.3, 192.8, 205.7;

Found C, 74.63; H, 6.07; N, 9.01%; M+1 (mass spectrum), 307.2. $C_{19}H_{18}N_2O_2$ requires C, 74.49; H, 5.92; N, 9.14%; M, 306.37.

3-acyl-1,5-benzodiazepine 5caa



Yield: 82%;

Characteristic: Pale yellow solid;

M.P.: 192-194 ℃;

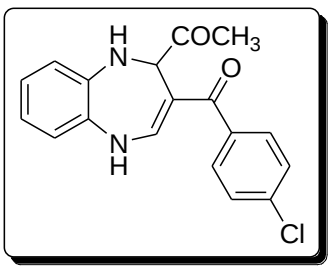
IR (KBr): 3328, 1696, 1642, 1538 cm^{-1};

^{1}H NMR (400 MHz, DMSO-d_6, TMS): δ 2.14 (3H, s, Me), 5.23 (1H, d, *J*=5.6 Hz, CH), 6.52 (1H, d, *J*=5.2, NH), 6.73-6.86 (4H, m, Ph), 7.09 (1H, d, *J*=8.4 Hz, CH), 7.26-7.54 (4H, m, Ph), 9.54 (1H, d, *J*=8.0 Hz, NH);

^{13}C NMR (100 MHz, DMSO-d_6, TMS): δ 28.6, 63.1, 110.5, 115.4, 115.6, 120.2, 120.6, 120.9, 123.9, 130.1, 131.0, 131.1, 137.1, 137.1, 138.4, 146.6, 162.1, 164.5, 191. 6, 205.7;

Found C, 69.80; H, 4.92; N, 8.88%; M+1 (mass spectrum), 311.2. $C_{18}H_{15}FN_2O_2$ requires C, 69.67; H, 4.87; N, 9.03%; M, 310.33.

3-acyl-1,5-benzodiazepine 5daa



Yield: 77%;

Characteristic: Yellow solid;

M.P.: 195-196 ℃;

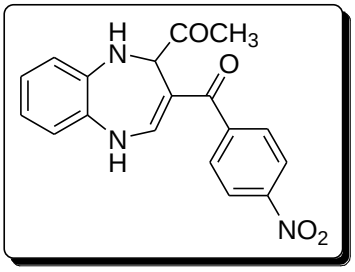
IR (KBr): 3340, 1702, 1635,1533 cm^{-1};

^{1}H NMR (400 MHz, DMSO-d_6, TMS): δ 2.14 (3H, s, Me), 5.22 (1H, d, *J*=5.6 Hz, CH), 6.54 (1H, d, *J*=6.0 Hz, NH), 6.71-6.88 (4H, m,Ph), 7.07 (1H, d, *J*=8.0 Hz, CH), 7.48-7.54 (4H, m, Ph), 9.57 (1H, d, *J*=8.0 Hz, NH);

^{13}C NMR (100 MHz, DMSO-d_6, TMS): δ 28.6, 63.0, 110.59, 120.3, 120.6, 120.9, 124.0, 128.7, 130.0, 130.5, 134.9, 138.4, 139.4, 146.7, 191.6, 205.6;

Found C, 66.33; H, 4.87; N, 8.46%; M+1 (mass spectrum), 327.2. $C_{18}H_{15}ClN_2O_2$ requires C, 66.16; H, 4.63; N, 8.57%; M, 326.78.

3-acyl-1,5-benzodiazepine 5eaa



Yield: 83%;

Characteristic: Tangerine solid;

M.P.: 191-192 ℃;

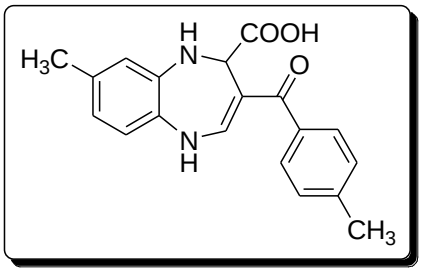
IR (KBr): 3334, 1702, 1635,1533 cm^{-1};

^{1}H NMR (400 MHz, DMSO-d_6, TMS): δ 2.15 (3H, s, Me), 5.27 (1H, d, *J*=4.8 Hz, CH), 6.59 (1H, d, *J*=5.6 Hz, NH), 6.83-6.89 (4H, m, Ph), 7.02 (1H, d, *J*=8.0 Hz, CH), 7.71-8.31 (4H, m, Ph), 9.71 (1H, d, *J*=8.4 Hz, NH);

^{13}C NMR (100 MHz, DMSO-d_6, TMS): δ 28.6, 62.8, 110.5, 120.4, 120.8, 120.9, 123.9, 124.3, 129.7, 129.7, 138.6, 146.9, 147.4, 148.3, 190.6, 205.5;

Found C, 63.95; H, 4.32; N, 12.56%; M+1 (mass spectrum), 338.2. $C_{18}H_{15}N_3O_4$ requires C, 64.09; H, 4.48; N, 12.46%; M, 337.34.

3-acyl-1,5-benzodiazepine 5bbb



Yield: 97%;

Characteristic: Pale yellow solid;

M.P.: 200-202 ℃;

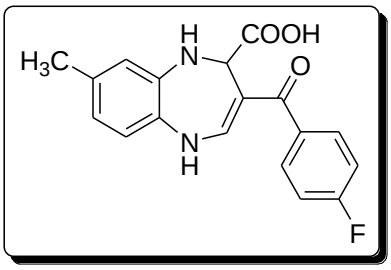
IR (KBr): 3357, 1709, 1605, 1573 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 2.18 (3H, s, Me), 2.37 (3H, s, Me), 5.14 (1H, d, *J*=4.5 Hz, CH), 6.21 (1H, d, *J*=4.5 Hz, NH), 6.56-6.73 (3H, m, Ph), 7.07 (1H, d, *J*=8.0 Hz, CH), 7.26-7.38 (4H, m, Ph), 9.38 (1H, d, *J*=8.5 Hz, NH), 12.19 (1H, s, COOH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 20.8, 21.4, 57.7, 110.9, 120.3, 121.3, 121.7, 128.3, 128.7, 129.1, 132.6, 138.0, 138.7, 139.9, 146.3, 172.9, 192.5;

Found C, 70.74; H, 5.59; N, 8.73%; M+1 (mass spectrum), 323.3. $C_{19}H_{18}N_2O_3$ requires C, 70.79; H, 5.63, N, 8.69%; M, 322.36.

3-acyl-1,5-benzodiazepine 5cbb



Yield: 92%;

Characteristic: Yellow solid;

M.P.: 196-198 ℃;

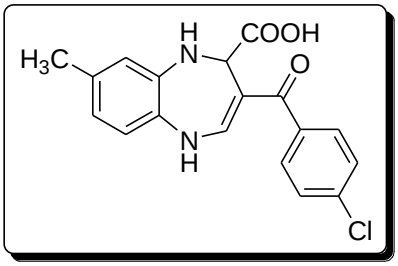
IR (KBr): 3357, 1717, 1629, 1597 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 2.18 (3H, s, Me), 5.15 (1H, d, *J*=2.5 Hz,

CH), 6.24 (1H, d, *J*=1.5 Hz, NH), 6.57-6.75 (3H, m, Ph), 7.05 (1H, d, *J*=8.0 Hz, CH), 7.27-7.55 (4H, m, Ph), 9.46 (1H, d, *J*=7.5 Hz, NH), 12.21 (1H, s, COOH); ^{13}C NMR (125 MHz, DMSO-d$_6$, TMS): δ 20.8, 57.7, 110.9, 115.4, 115.6, 120.4, 121.4, 121.7, 128.3, 131.0, 131.1, 132.8, 138.7, 146.5, 172.9, 191.2;

Found C, 66.39; H, 4.77; N, 8.45%; M+1 (mass spectrum), 327.3. $C_{19}H_{18}N_2O_3$ requires C, 66.25; H, 4.63; N, 8.58%; M, 326.33.

3-acyl-1,5-benzodiazepine 5dbb



Yield: 91%;

Characteristic: Yellow solid;

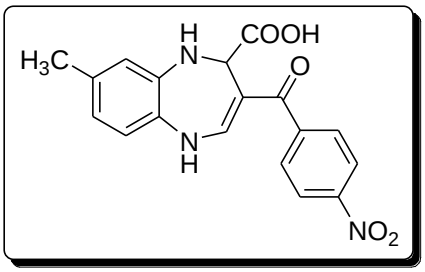
M.P.: 190-192 ℃;

IR (KBr): 3341, 1693, 1629, 1534 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d$_6$, TMS): δ 2.18 (3H, s, Me), 5.13 (1H, d, *J*=5.0 Hz, CH), 6.24 (1H, d, *J*=5.5 Hz, NH), 6.56-6.74 (3H, m, Ph), 7.02 (1H, d, *J*=8.5 Hz, CH), 7.46-7.53 (4H, m, Ph), 9.46 (1H, d, *J*=8.0 Hz, NH), 12.18 (1H, s, COOH); ^{13}C NMR (125 MHz, DMSO-d$_6$, TMS): δ 20.8, 57.6, 111.0, 120.5, 121.4, 121.7, 128.2, 128.6, 130.4, 132.9, 134.8, 138.7, 139.6, 146.6, 172.8, 191.1;

Found C, 63.11; H, 4.49; N, 8.09%; M+1 (mass spectrum), 343.2. $C_{18}H_{15}ClN_2O_3$ requires C, 63.07; H, 4.41; N, 8.17%; M, 342.78.

3-acyl-1,5-benzodiazepine 5ebb



Yield: 95%;

Characteristic: Red solid;

M.P.: 196-198 ℃;

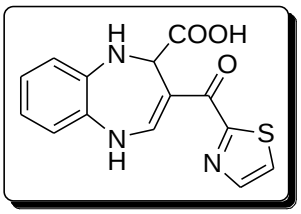
IR (KBr): 3349, 1693, 1645, 1541 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 2.18 (3H, s, Me), 5.18 (1H, d, *J*=5.0 Hz, CH), 6.30 (1H, d, *J*=5.5 Hz, NH), 6.58-6.76 (3H, m, Ph), 6.97 (1H, d, *J*=8.5 Hz, CH), 7.68-8.31 (4H, m, Ph), 9.59 (1H, d, *J*=8.5 Hz, NH), 12.24 (1H, s, COOH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 20.8, 57.4, 111.1, 120.7, 121.5, 121.8, 123.9, 128.0, 129.7, 133.2, 138.9, 147.2, 147.3, 148.3, 172.7, 190.1;

Found C, 61.21; H, 4.37; N, 11.81%; M+1 (mass spectrum), 354.3. $C_{18}H_{15}N_3O_5$ requires C, 61.19; H, 4.28; N, 11.89%; M, 353.33.

3-acyl-1,5-benzodiazepine 5fab



Yield: 95%;

Characteristic: Deep yellow solid;

M.P.: 118-120 ℃;

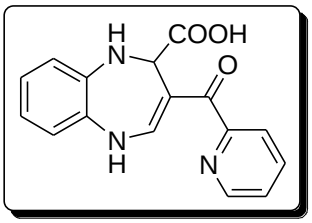
IR (KBr): 3302, 1684, 1629, 1534 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 5.21 (1H, d, *J*=3.5 Hz, CH), 6.42 (1H, d, *J*=6.0 Hz, NH), 6.77-6.93 (4H, m, Ph), 8.00-8.03 (2H, m, thiazole ring), 9.19 (1H, d, *J*=6.5 Hz, CH), 10.12 (1H, d, *J*=8.5 Hz, NH), 12.24 (1H, s, COOH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 57.9, 109.8, 120.7, 120.8, 121.4, 124.4, 125.6, 130.5, 139.2, 144.2, 148.2, 171.0, 172.7, 177.0;

Found C, 55.71; H, 3.53; N, 14.10%; M-1 (mass spectrum), 300.1. $C_{14}H_{11}N_3O_3S$ requires C, 55.80; H, 3.68; N, 13.95%; M, 301.32.

3-acyl-1,5-benzodiazepine 5gab



Yield: 93%;

Characteristic: Brown solid;

M.P.: 200-202 ℃;

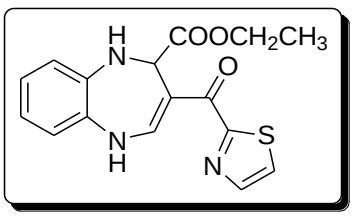
IR (KBr): 3357, 1701, 1629, 1581 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 5.22 (1H, d, *J*=2.0 Hz, CH), 6.35 (1H, d, *J*=2.5 Hz, NH), 6.74-7.66 (5H, m, Pyridine ring), 7.79 (1H, d, *J*=8.0 Hz, CH), 7.91-8.61 (4H, m, Ph), 9.68 (1H, d, *J*=8.0 Hz, NH), 12.20 (1H, s, COOH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 57.6, 110.6, 120.5, 120.6, 121.4, 123.9, 124.0, 125.1, 130.7, 137.7, 139.0, 148.0, 148.2, 158.3, 172.9, 188.7;

Found C, 65.22; H, 4.61; N, 14.01%; M+1 (mass spectrum), 295.9. $C_{16}H_{13}N_3O_3$ requires C, 65.08; H, 4.44; N, 14.23%; M, 295.30.

3-acyl-1,5-benzodiazepine 5fac



Yield: 92%;

Characteristic: Yellow solid;

M.P.: 164-166 ℃;

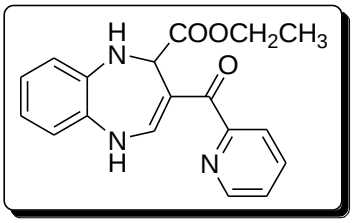
IR (KBr): 3318, 1709, 1629, 1522 cm^{-1};

^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 0.94 (3H, t, *J*=7.0, Me), 3.90 (2H, q, *J*=2.5, CH_2), 5.25 (1H, d, *J*=4.5 Hz, CH), 6.53 (1H, d, *J*=6.0 Hz, NH), 6.95-8.04 (6H, m, Ph), 8.01-8.04 (2H, m, thiazole ring), 9.23 (1H, d, *J*=7.0 Hz, CH), 10.18 (1H, d, *J*=8.5 Hz, NH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 14.5, 57.9, 60.6, 109.1, 120.9, 121.0, 121.3, 124.5, 125.7, 130.8, 138.8, 144.2, 148.4, 170.8, 171.1, 177.0;

Found C, 58.27; H, 4.41; N, 12.85%; M+1 (mass spectrum), 330.2. $C_{16}H_{15}N_3O_3S$ requires C, 58.34; H, 4.59; N, 12.76%; M, 329.37.

3-acyl-1,5-benzodiazepine 5gac



Yield: 89%;

Characteristic: Pale gray solid;

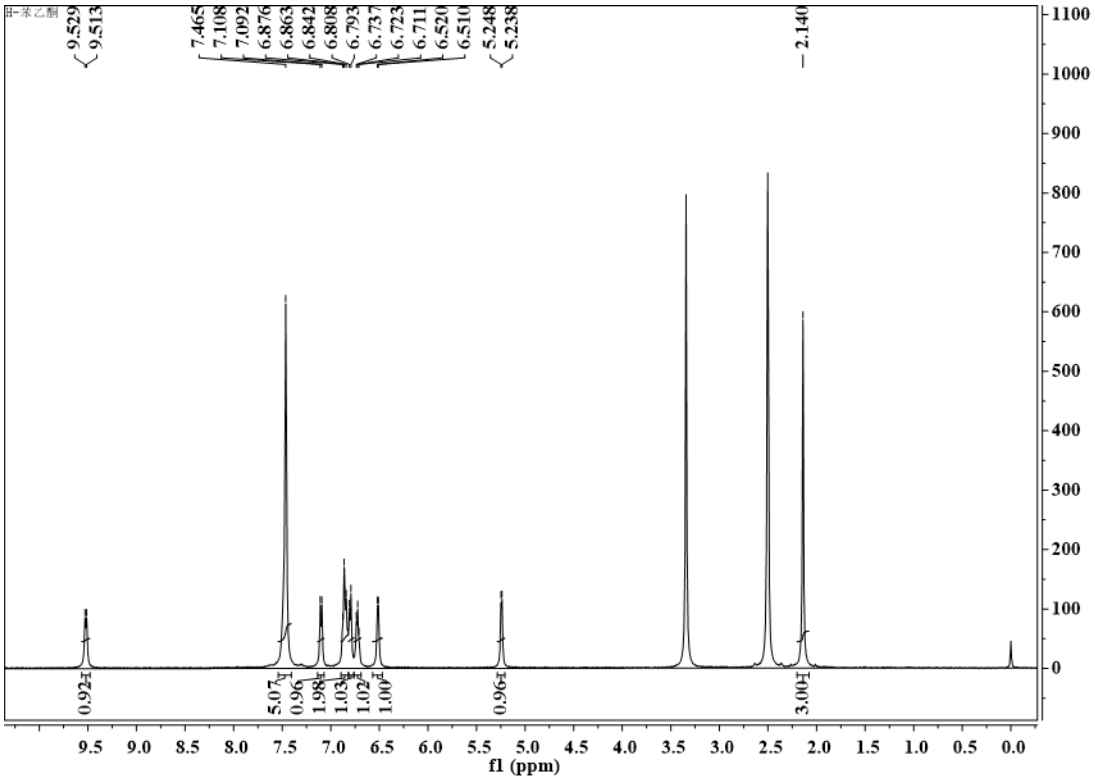
M.P.: 94-96 ℃;

IR (KBr): 3318, 1717, 1645, 1526 cm^{-1};

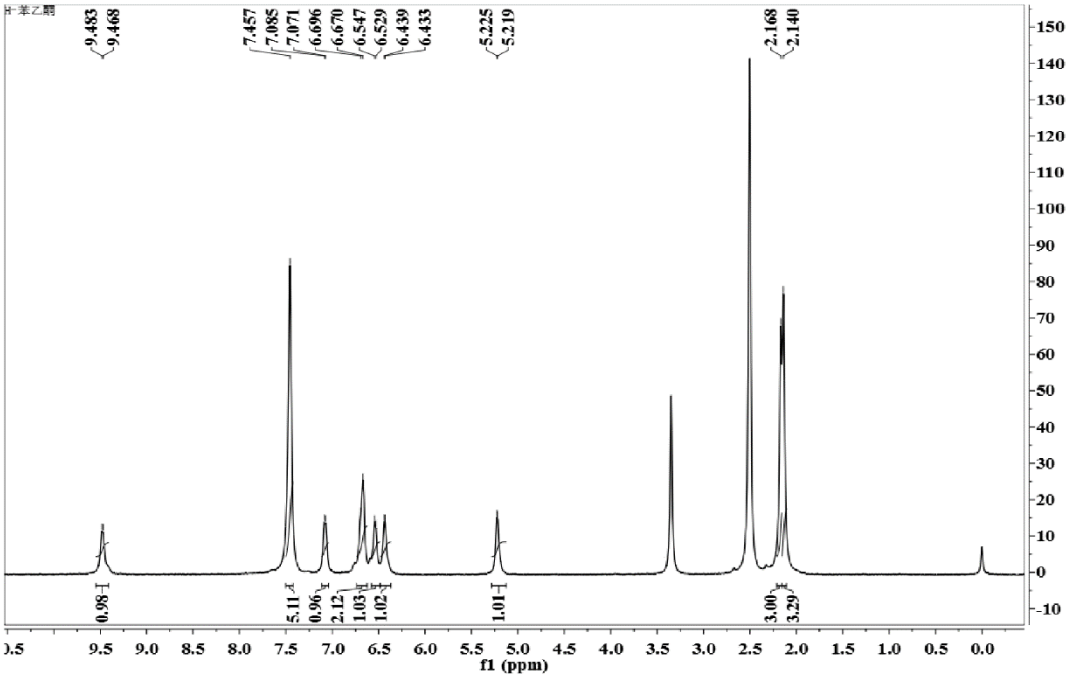
^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ 0.96 (3H, t, *J*=7.0, Me), 3.91 (2H, q, *J*=5.5, CH_2), 5.23 (1H, d, *J*=5.5 Hz, CH), 6.44 (1H, d, *J*=5.5 Hz, NH), 6.76-7.66 (5H, m, Pyridine ring), 7.83 (1H, d, *J*=8.5 Hz, CH), 7.92-8.61 (4H, m, Ph), 9.72 (1H, d, *J*=8.5 Hz, NH);

^{13}C NMR (125 MHz, DMSO-d_6, TMS): δ 14.6, 57.7, 60.5, 109.9, 120.5, 120.9, 121.3, 123.9, 124.0, 125.1, 131.0, 137.7, 138.6, 148.1, 148.2, 158.1, 171.3, 188.5;

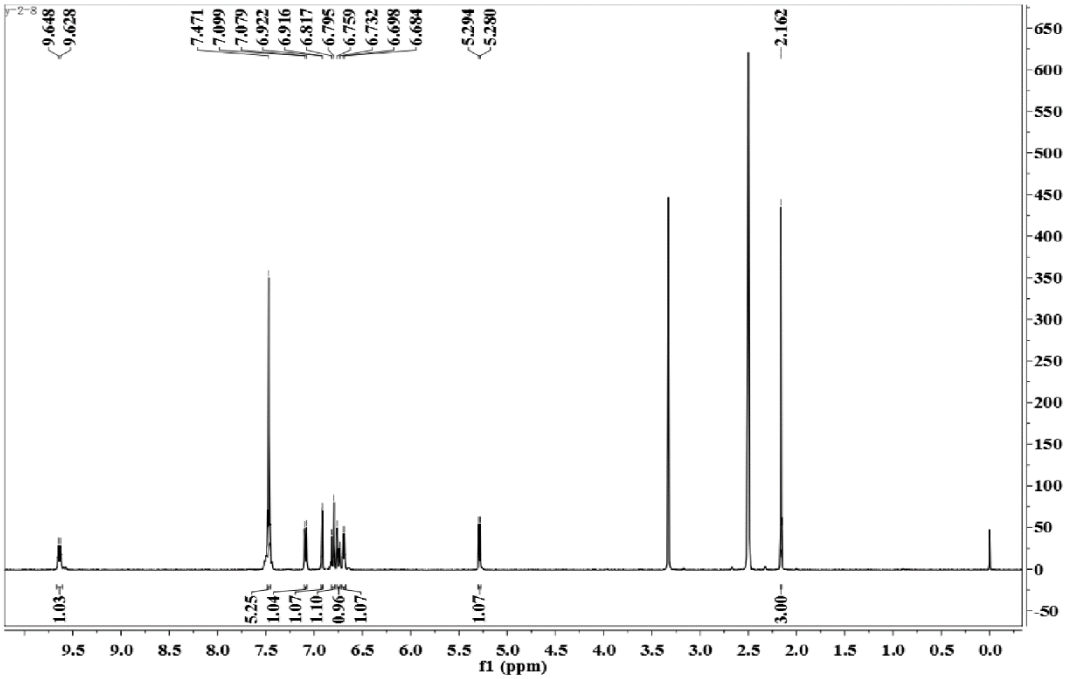
Found C, 66.79; H, 5.16; N, 13.23%; M+1 (mass spectrum), 323.9. $C_{18}H_{17}N_3O_3$ requires C, 66.86; H, 5.30; N, 13.00%; M, 323.35.



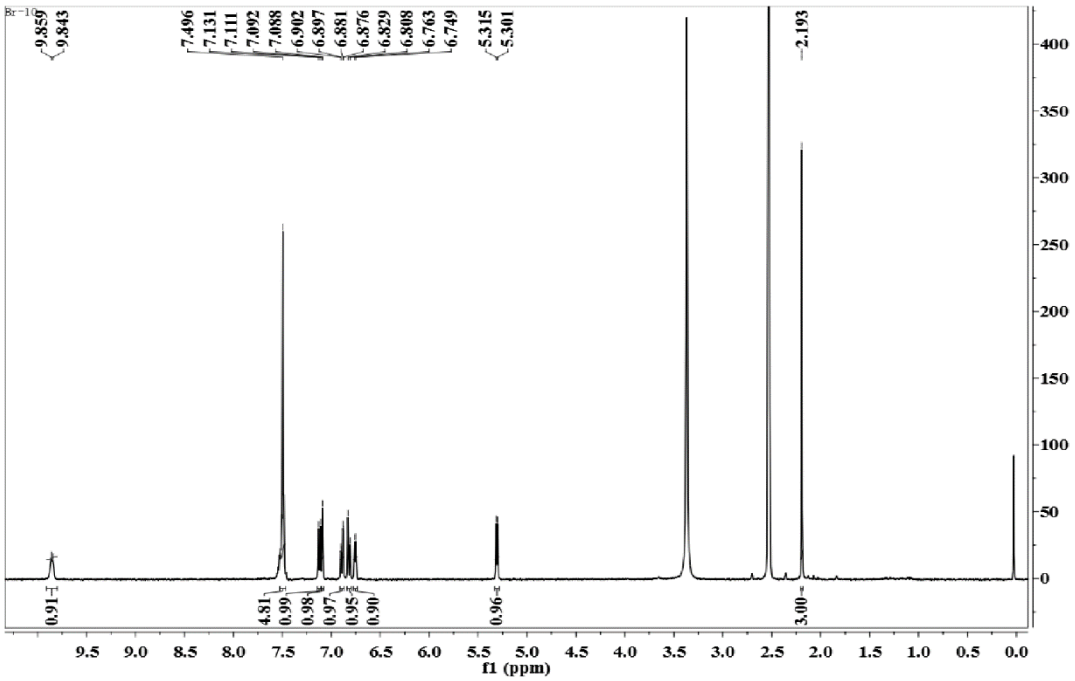
^{1}H NMR spectra of compound **5aaa**



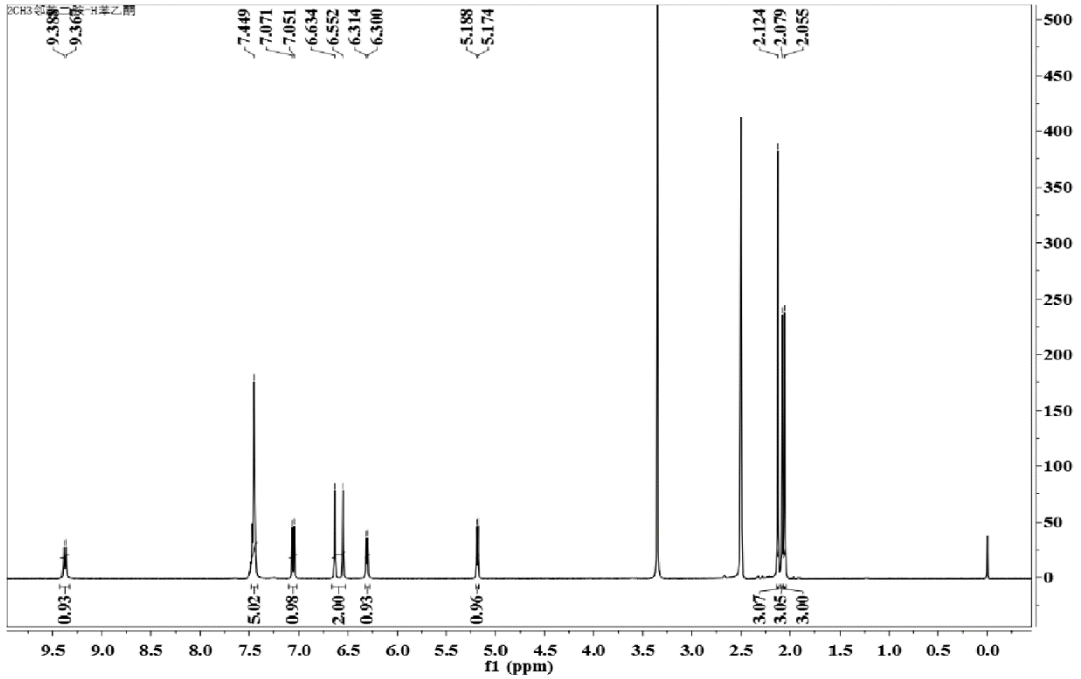
^{1}H NMR spectra of compound **5aba**



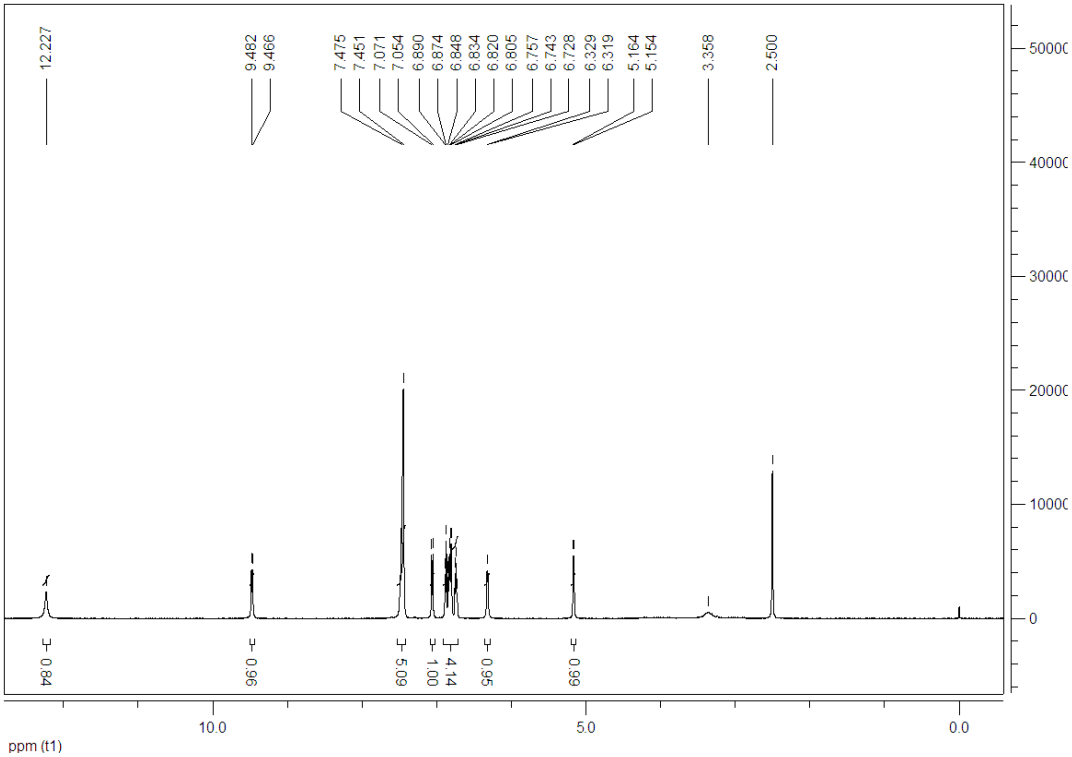
^{1}H NMR spectra of compound **5aca**



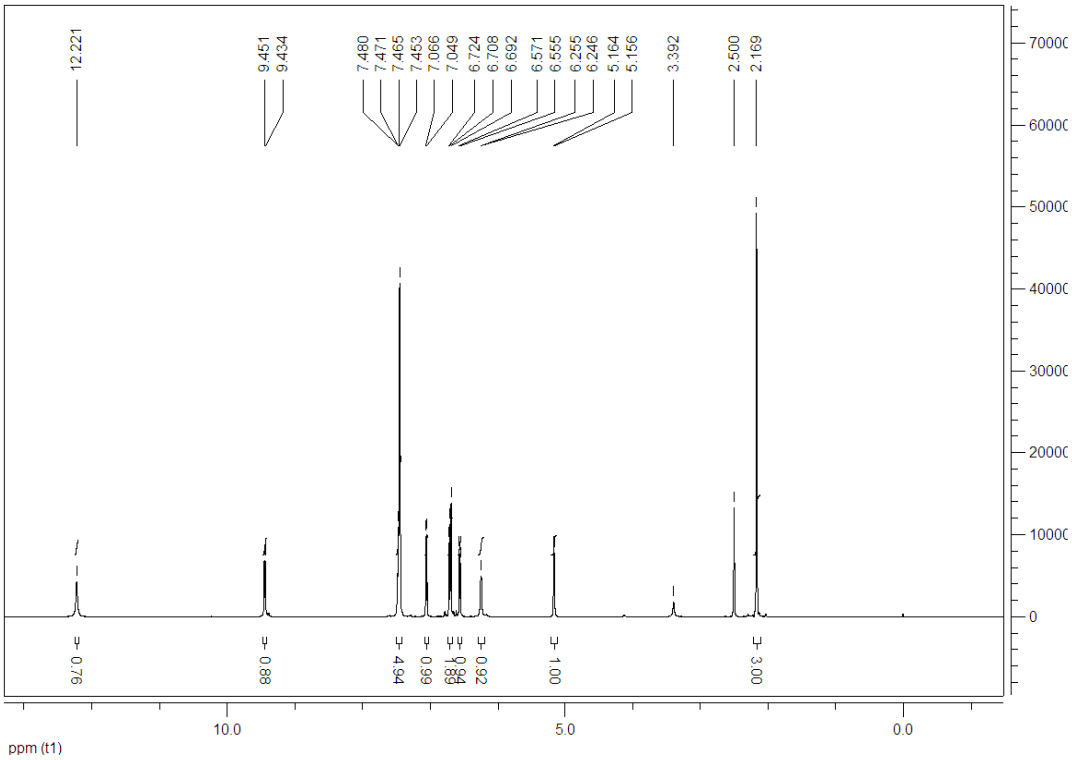
^{1}H NMR spectra of compound **5ada**



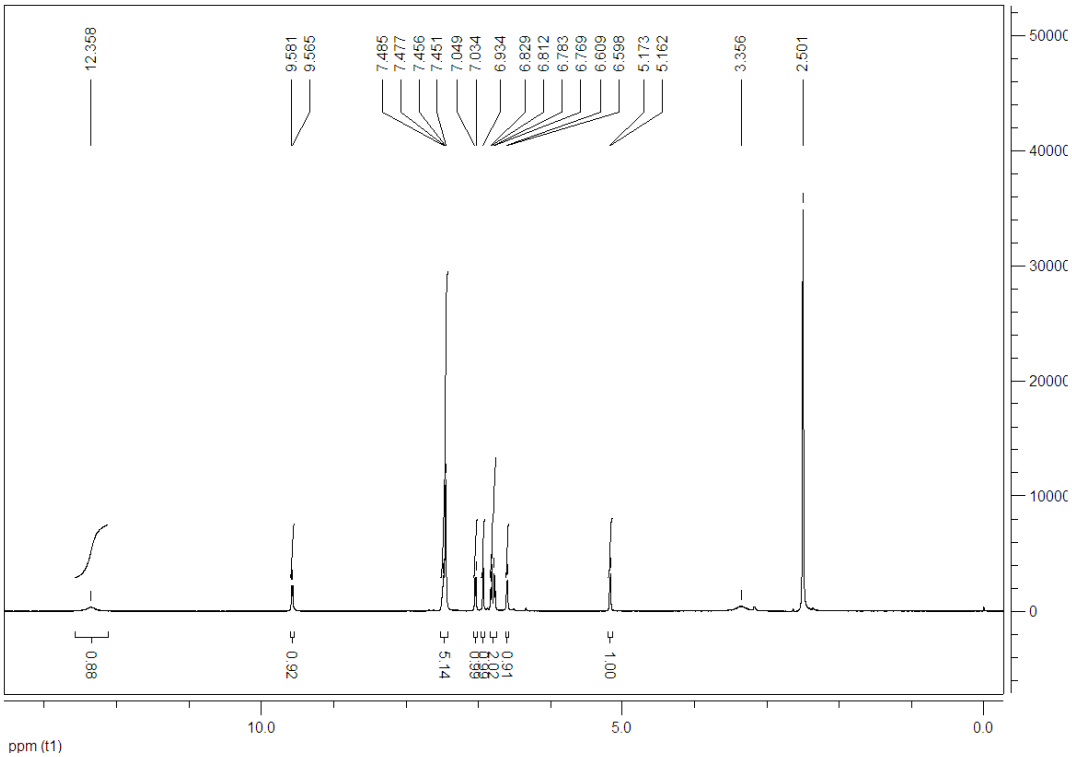
^{1}H NMR spectra of compound **5aea**



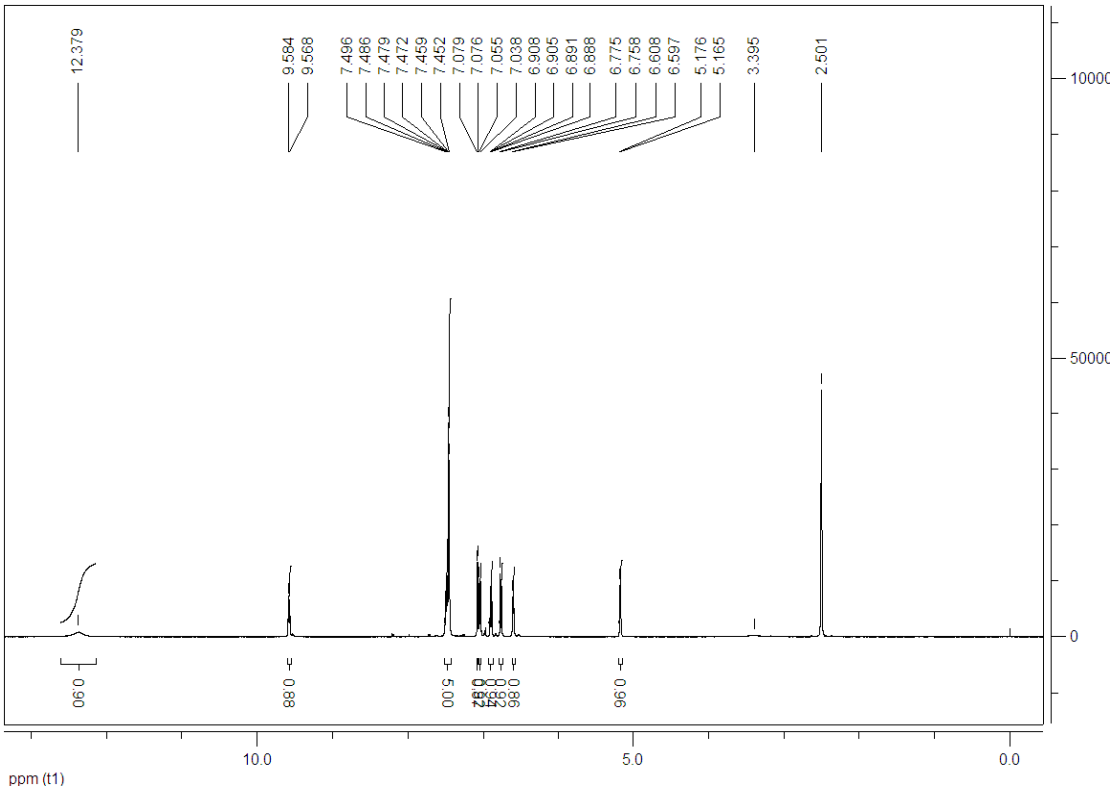
^{1}H NMR spectra of compound **5aab**



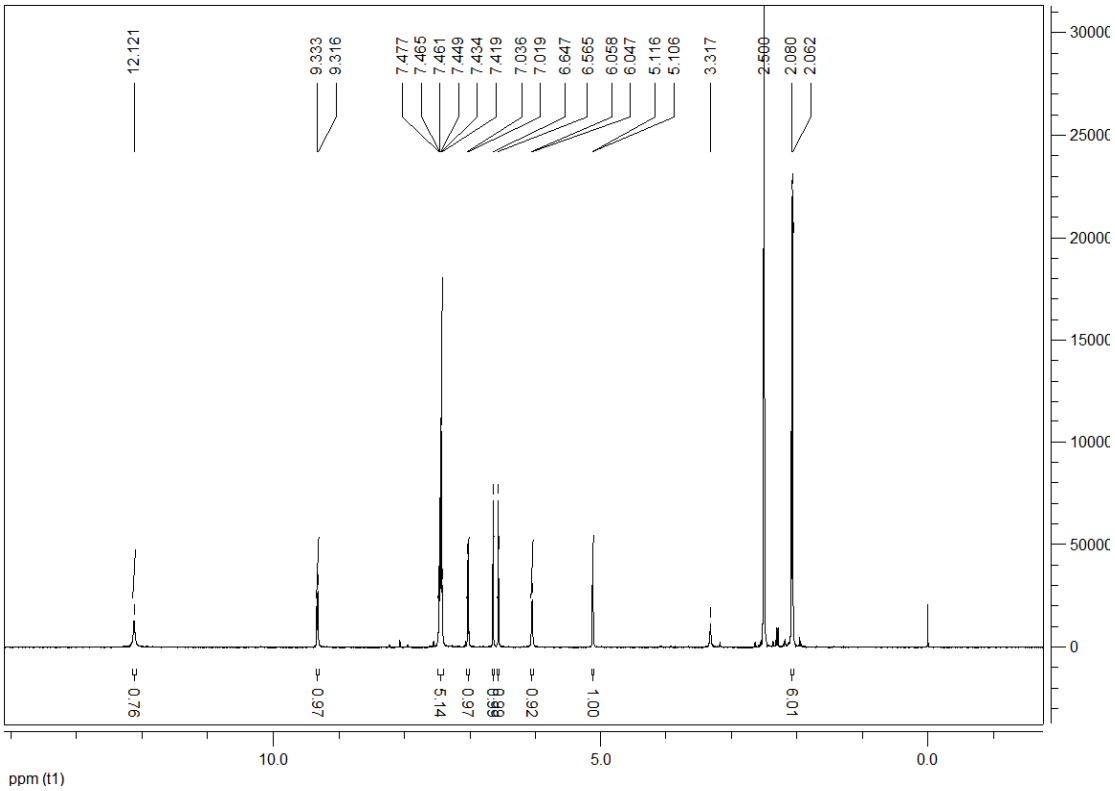
^{1}H NMR spectra of compound **5abb**



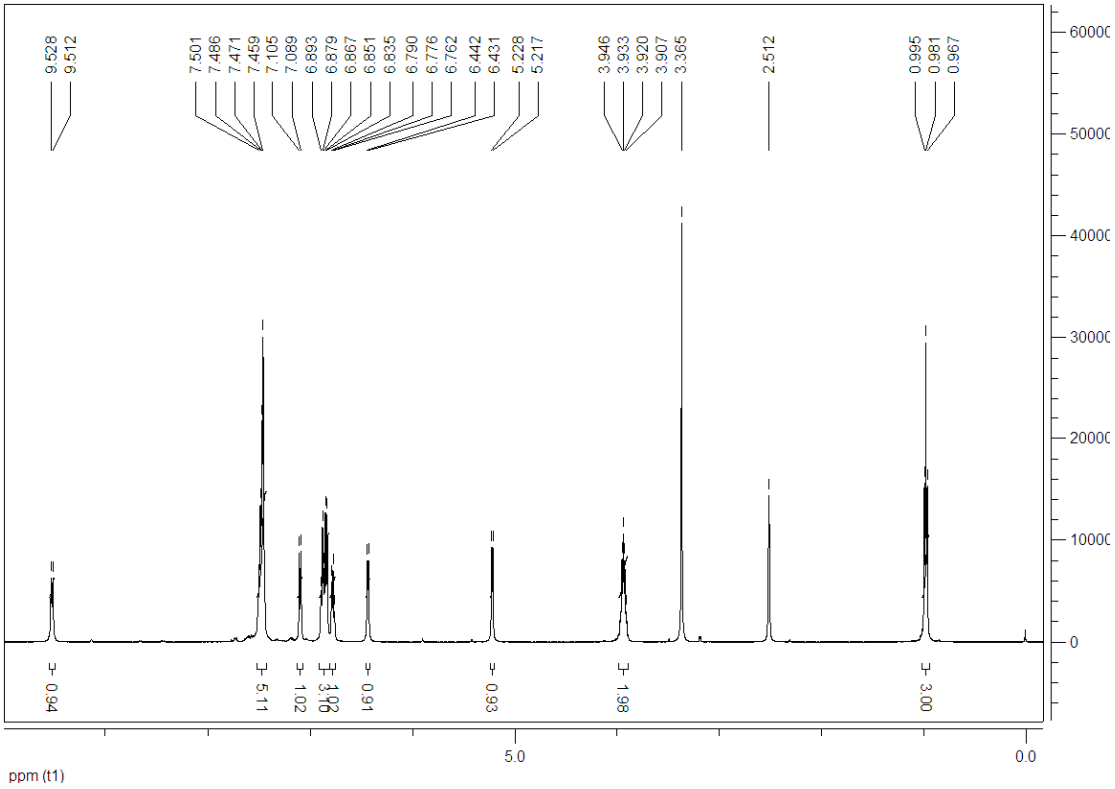
^{1}H NMR spectra of compound **5acb**



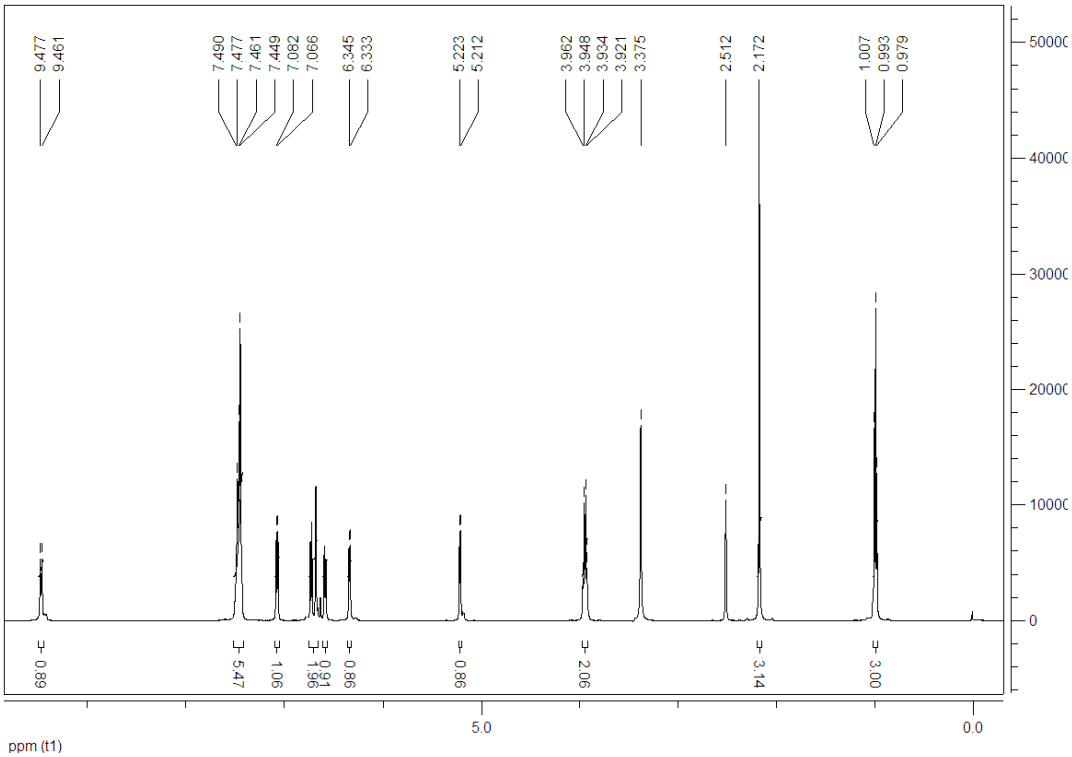
^{1}H NMR spectra of compound **5adb**



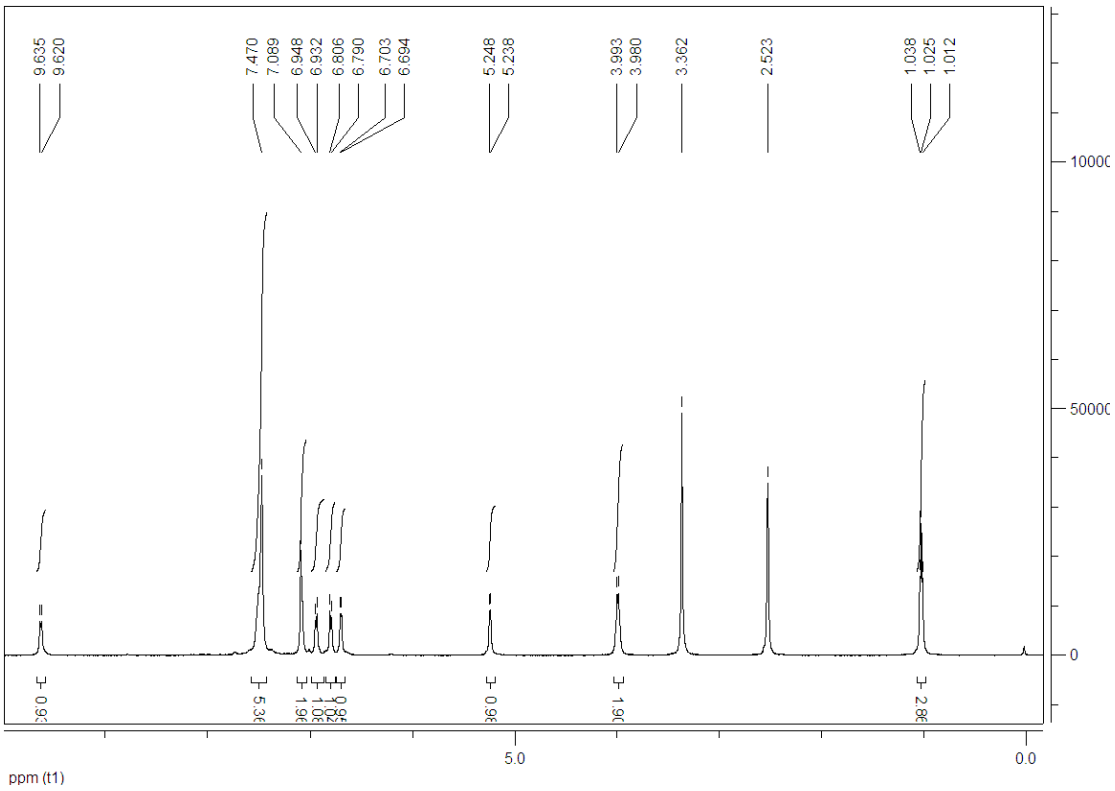
^{1}H NMR spectra of compound **5aeb**



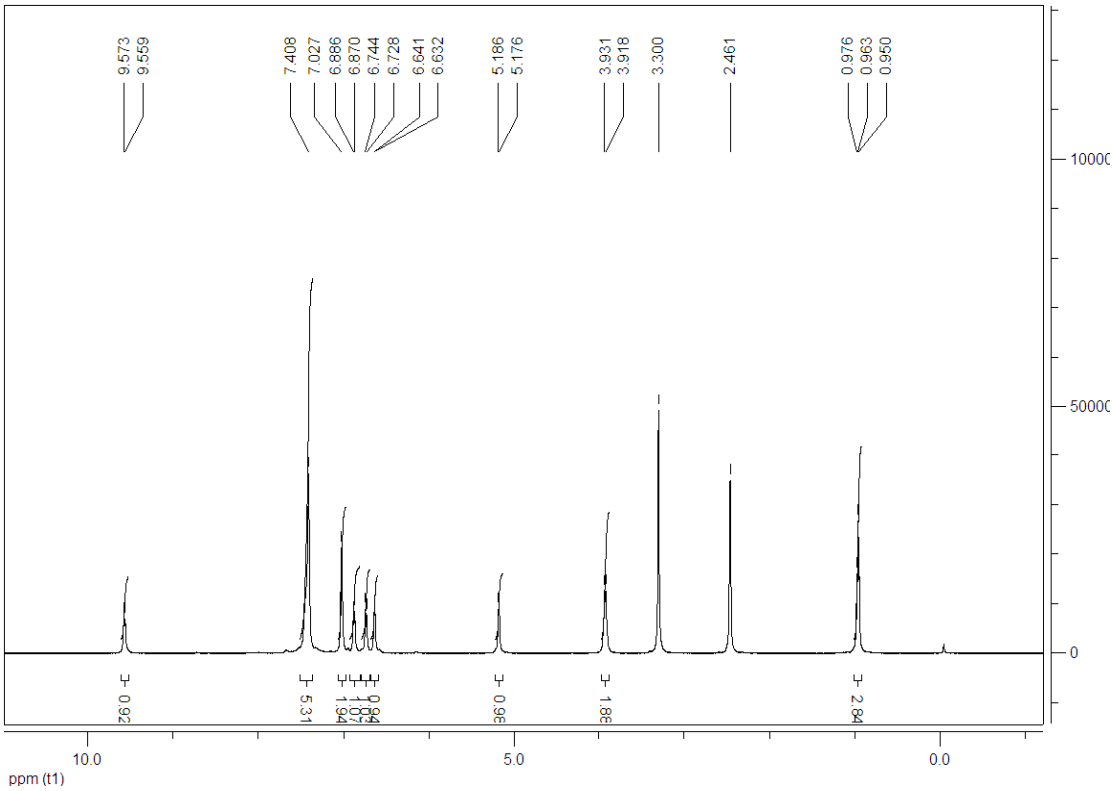
^{1}H NMR spectra of compound **5aac**



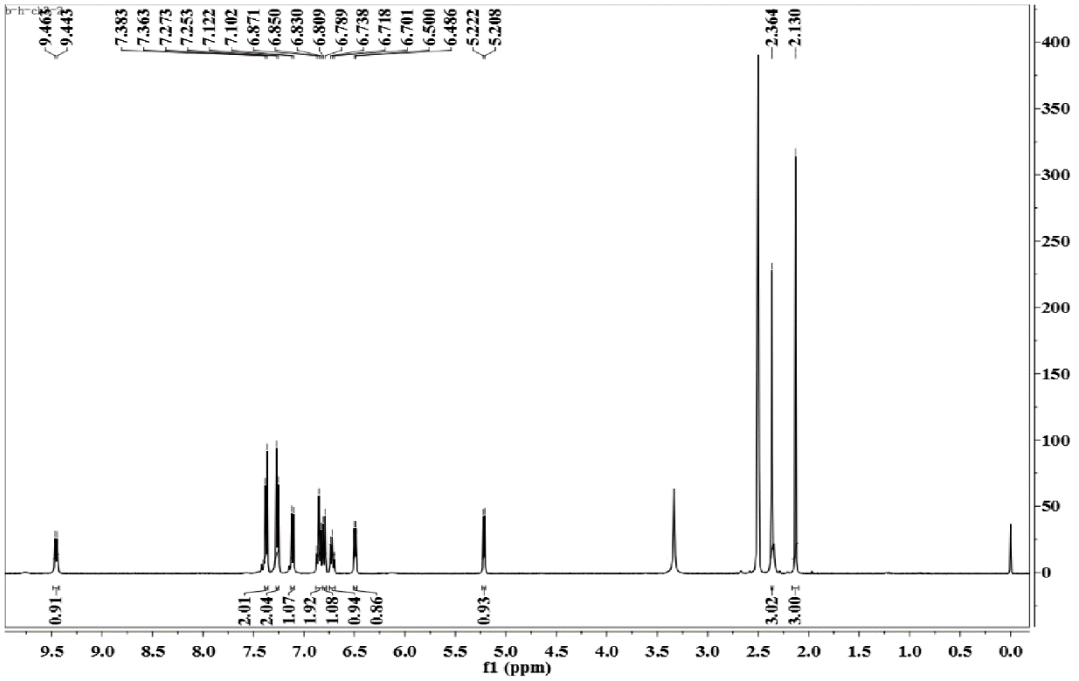
^{1}H NMR spectra of compound **5abc**



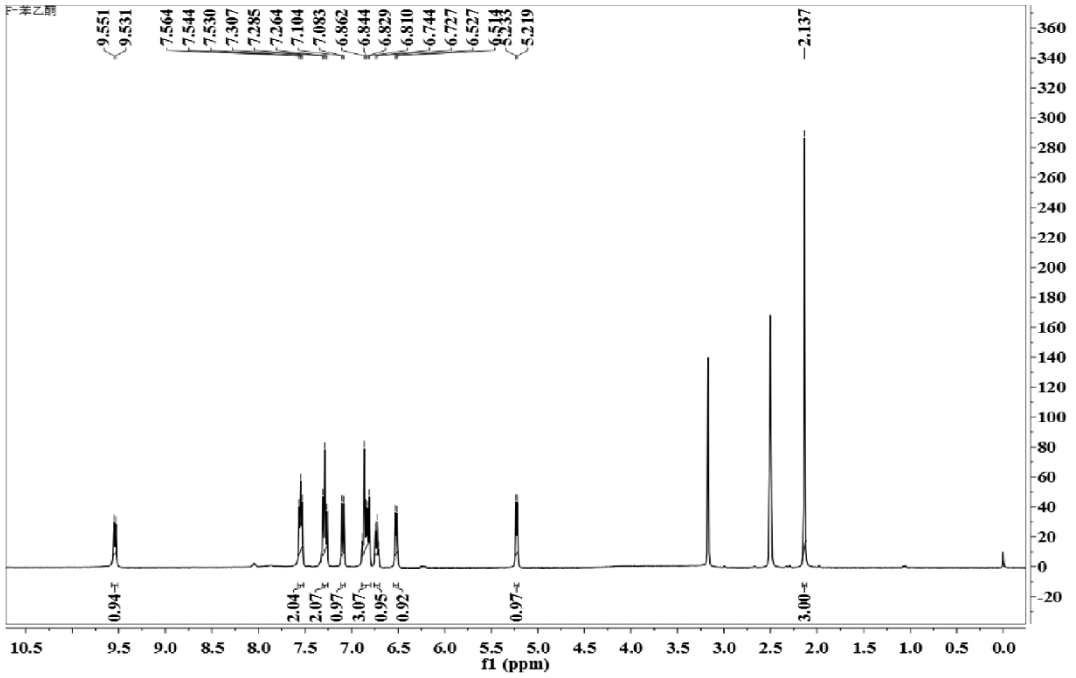
^{1}H NMR spectra of compound **5acc**



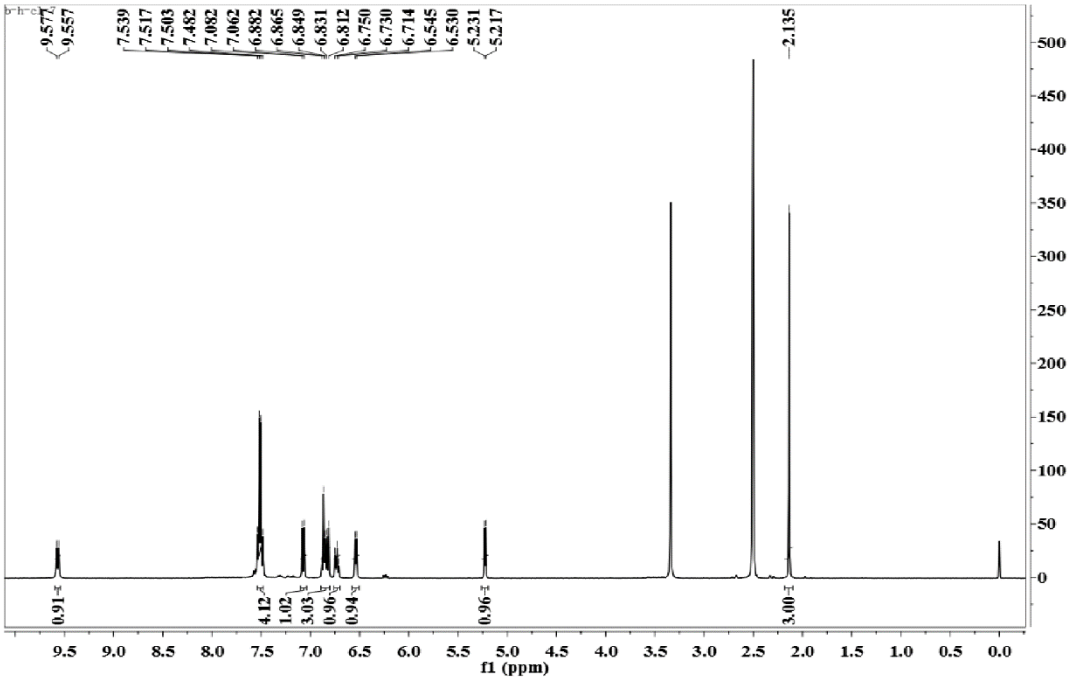
^{1}H NMR spectra of compound **5adc**



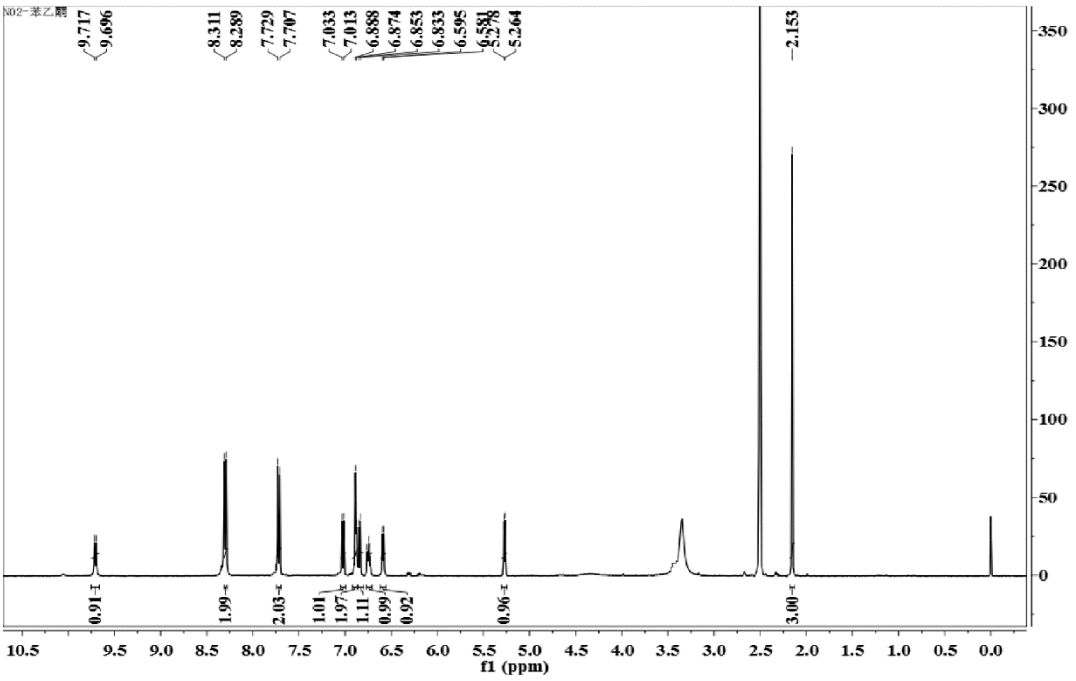
^{1}H NMR spectra of compound **5baa**



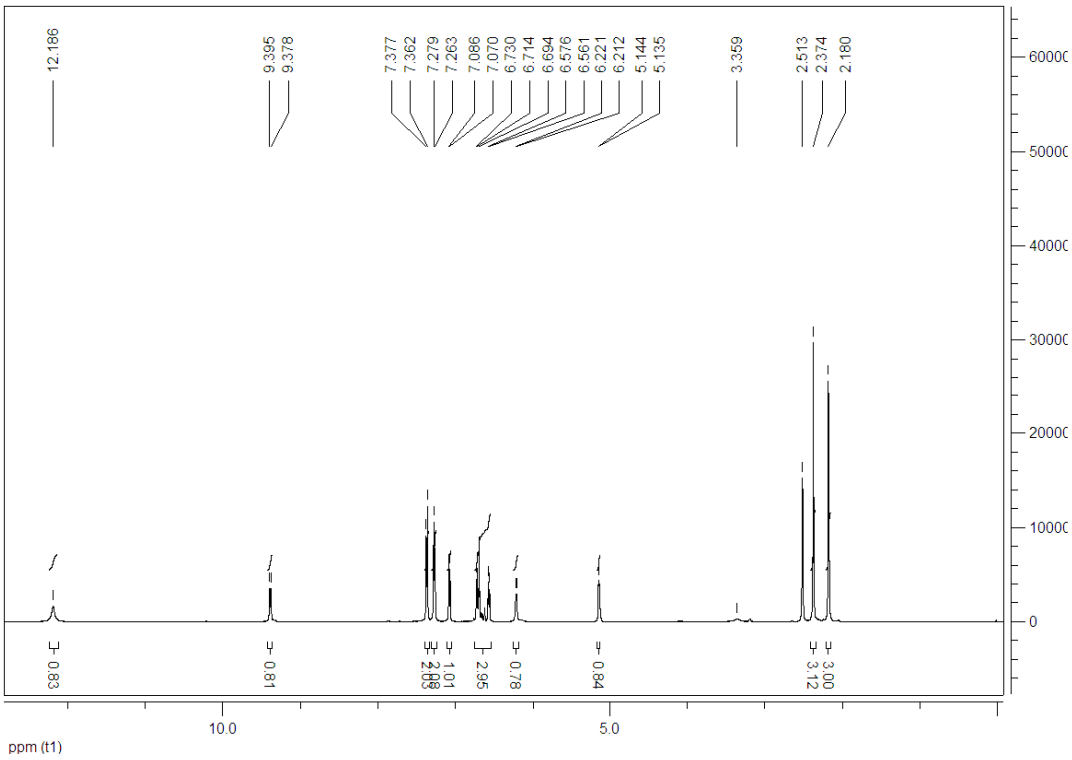
^{1}H NMR spectra of compound **5caa**



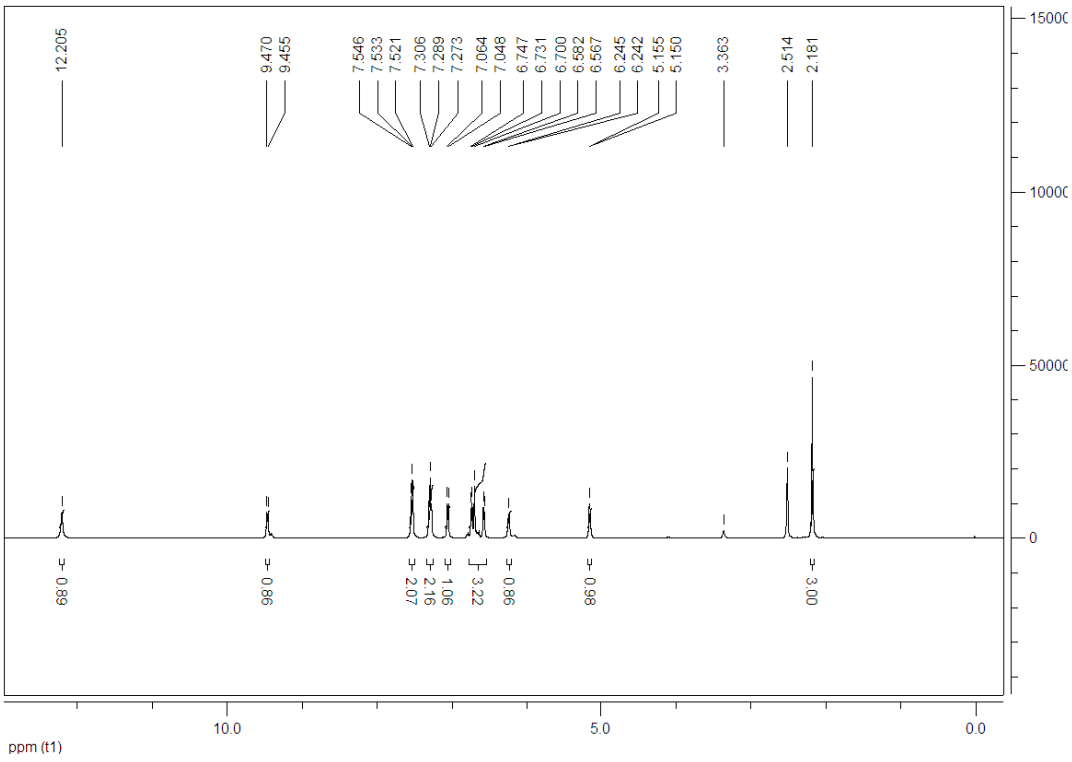
^{1}H NMR spectra of compound **5daa**



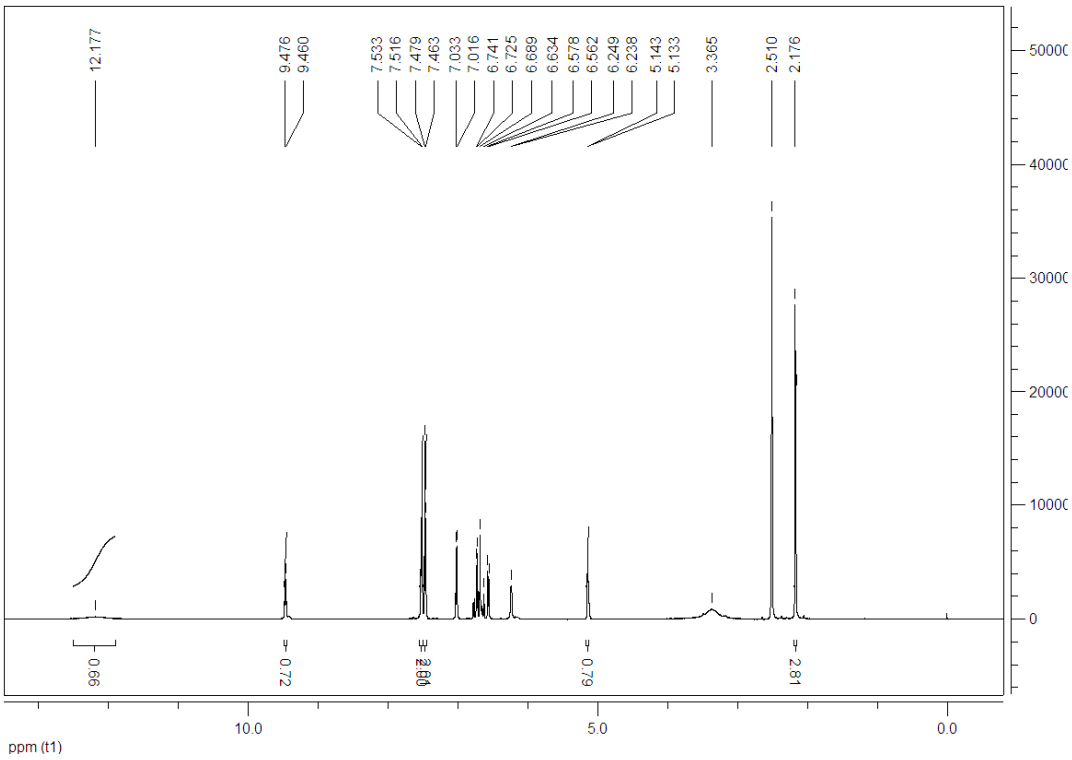
^{1}H NMR spectra of compound **5eaa**



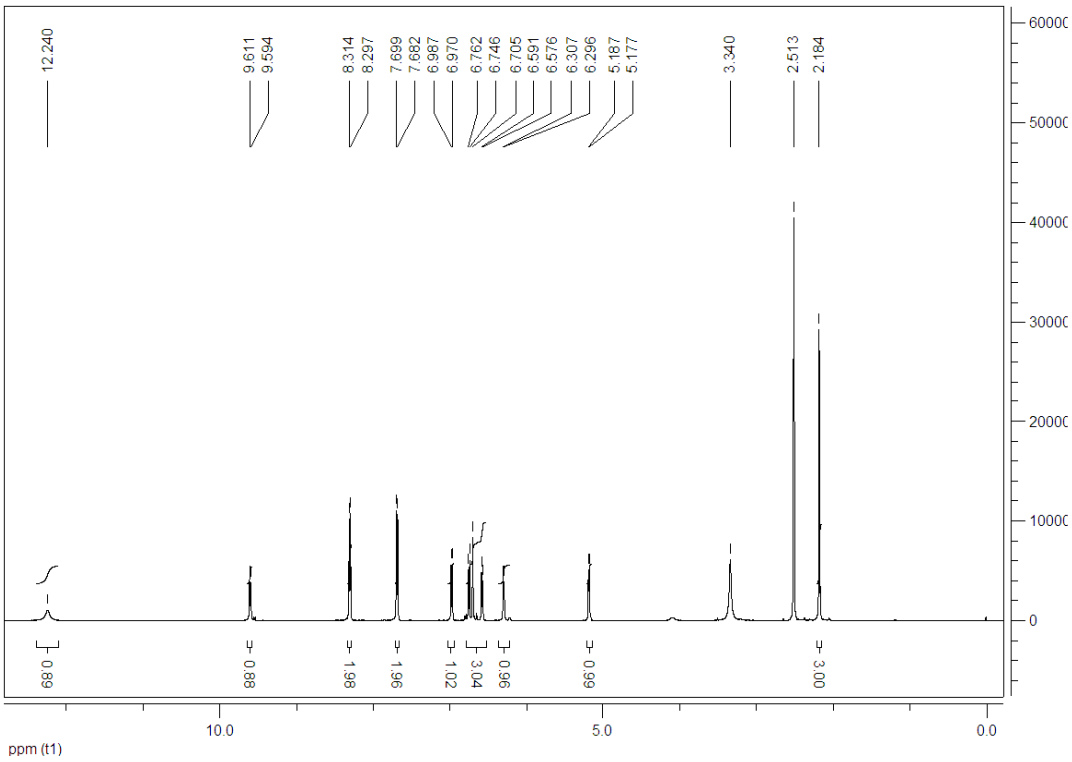
^{1}H NMR spectra of compound **5bbb**



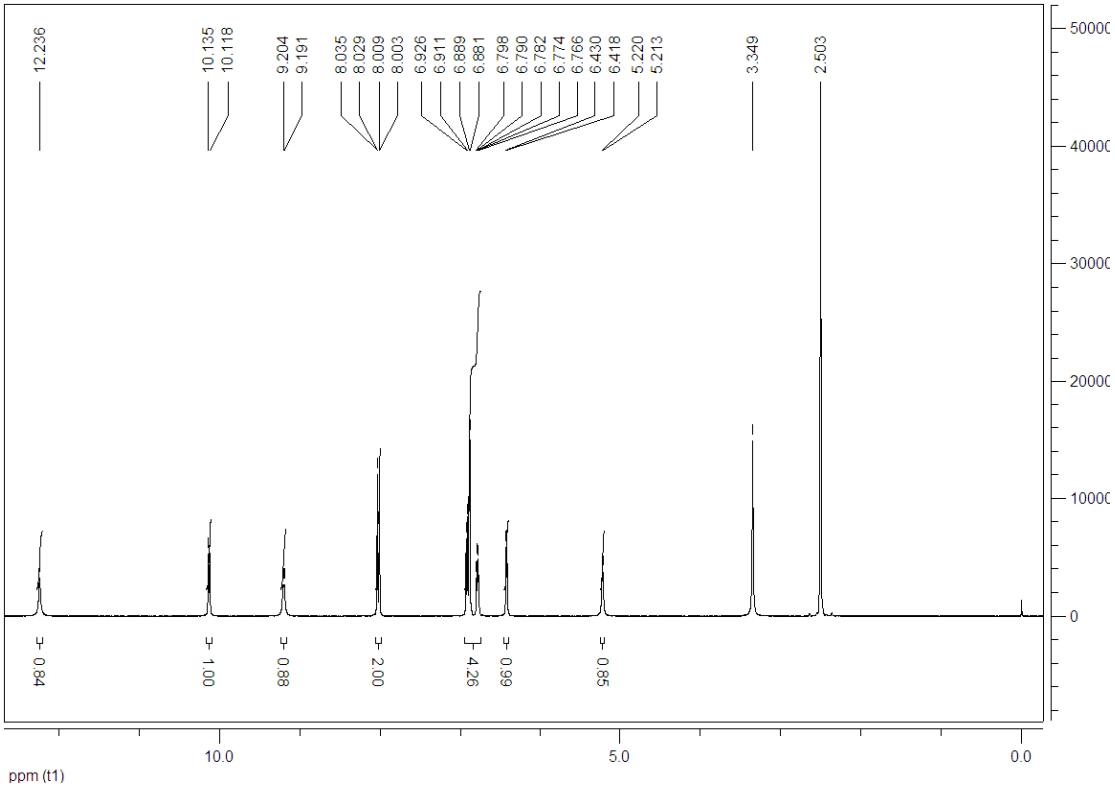
^{1}H NMR spectra of compound **5cbb**



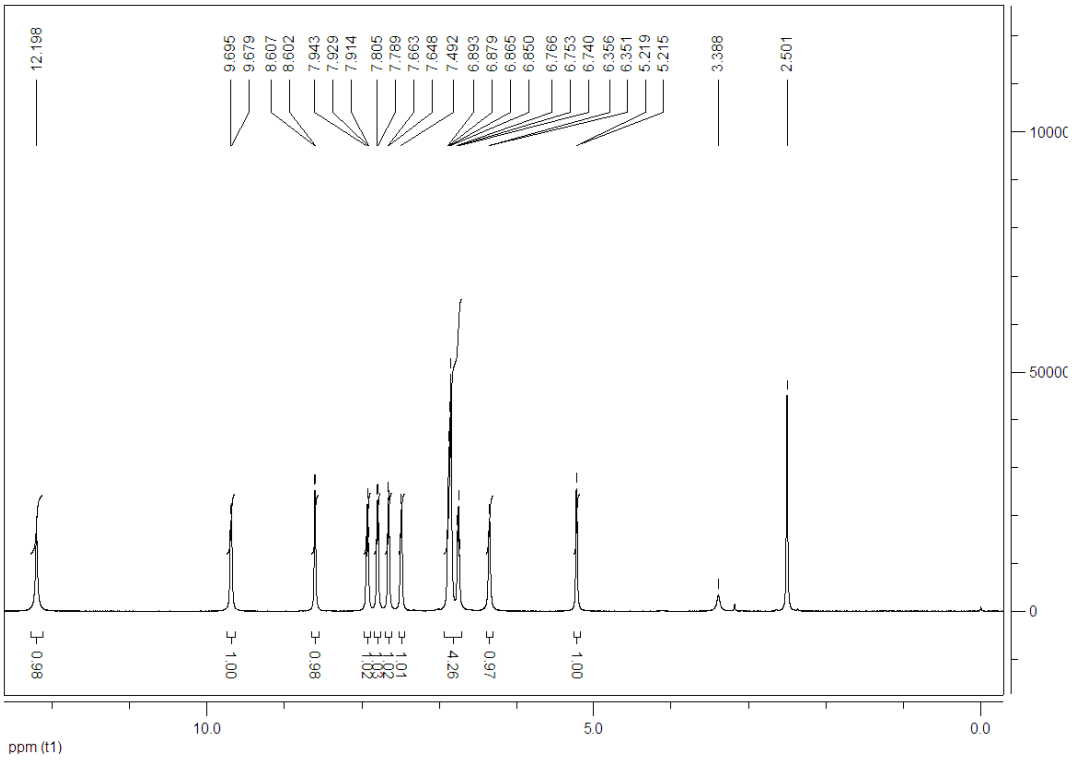
^{1}H NMR spectra of compound **5dbb**



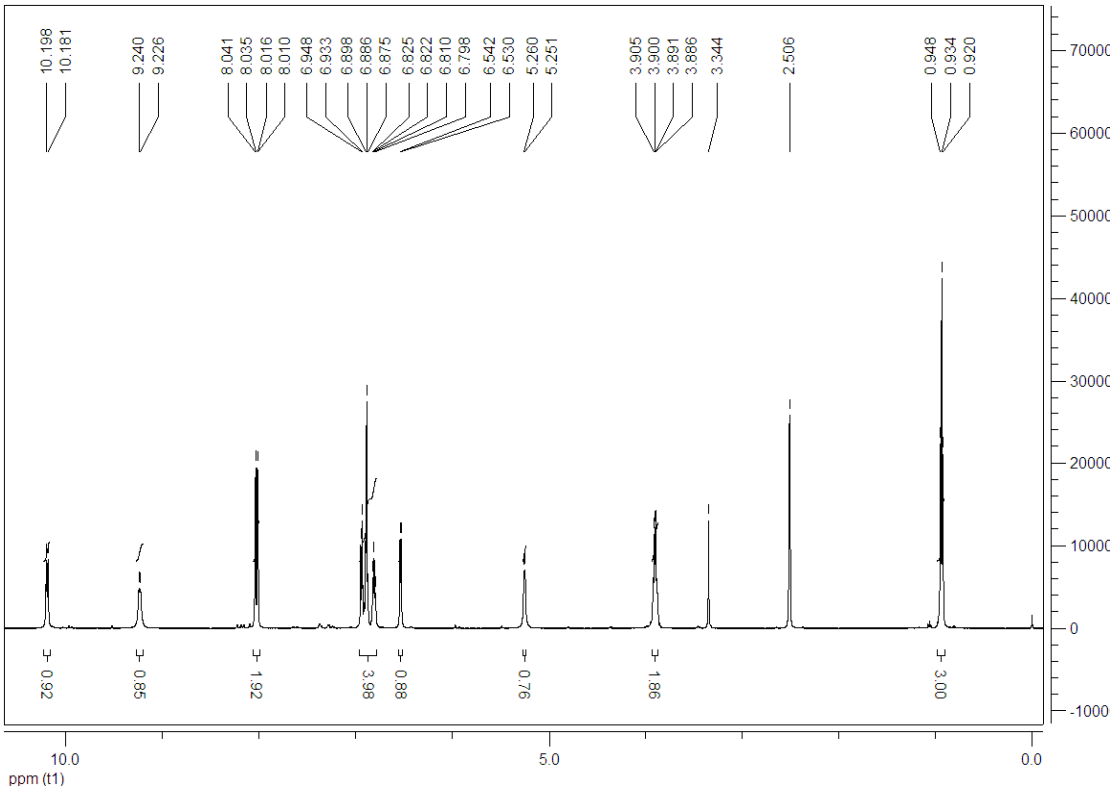
^{1}H NMR spectra of compound **5ebb**



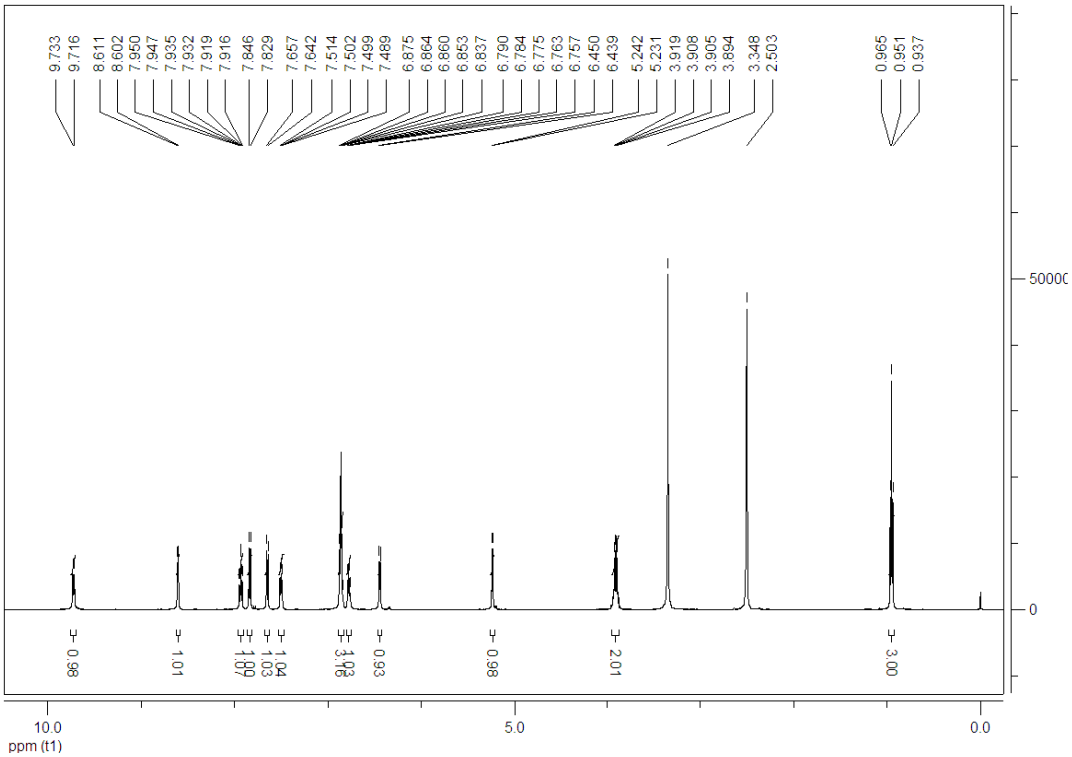
^{1}H NMR spectra of compound **5fab**



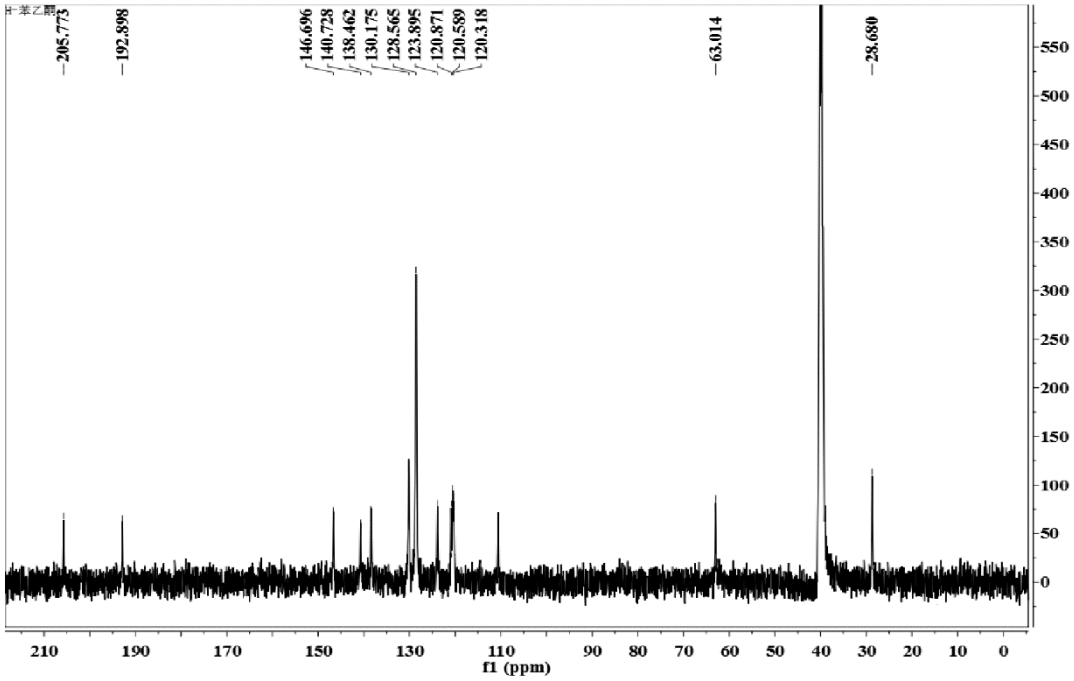
^{1}H NMR spectra of compound **5gab**



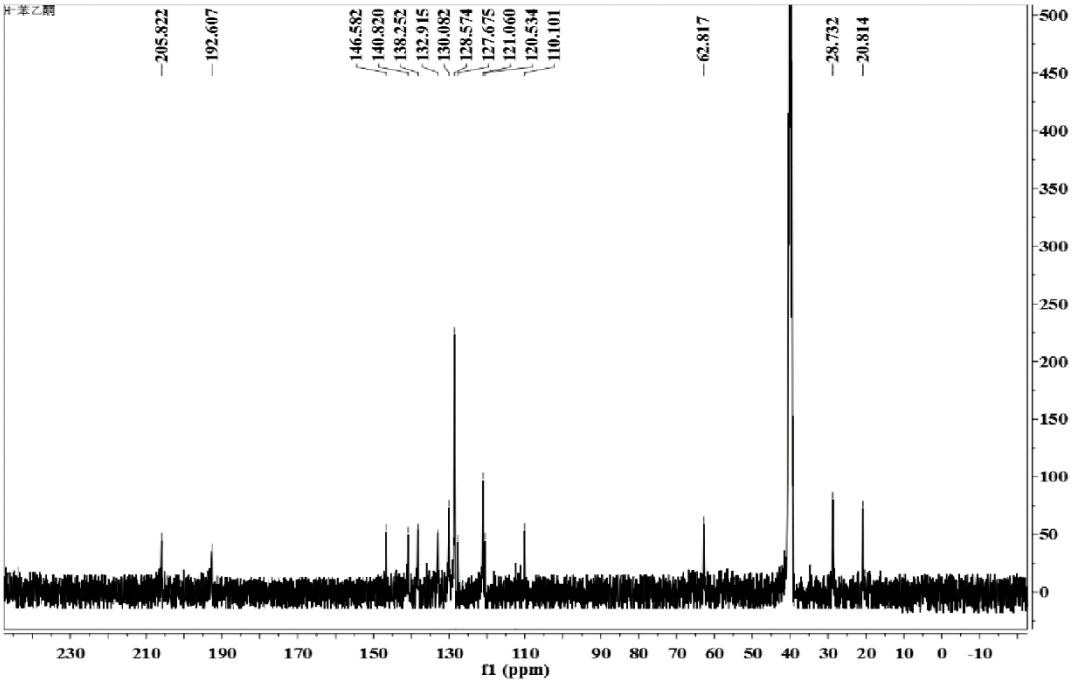
^{1}H NMR spectra of compound **5fac**



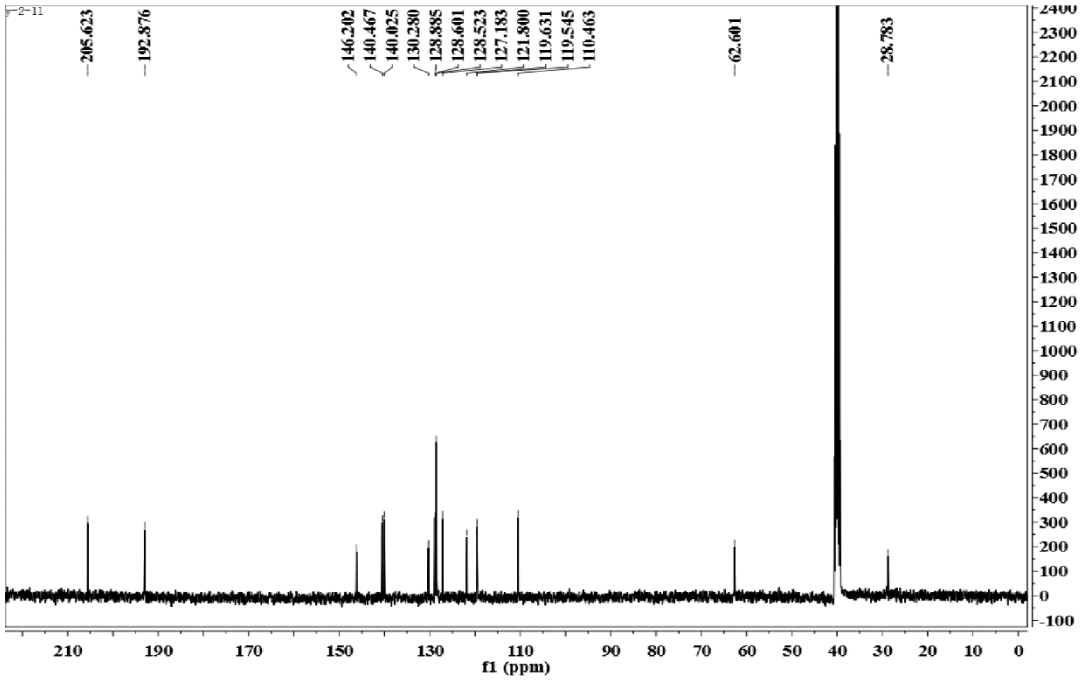
^{1}H NMR spectra of compound **5gac**



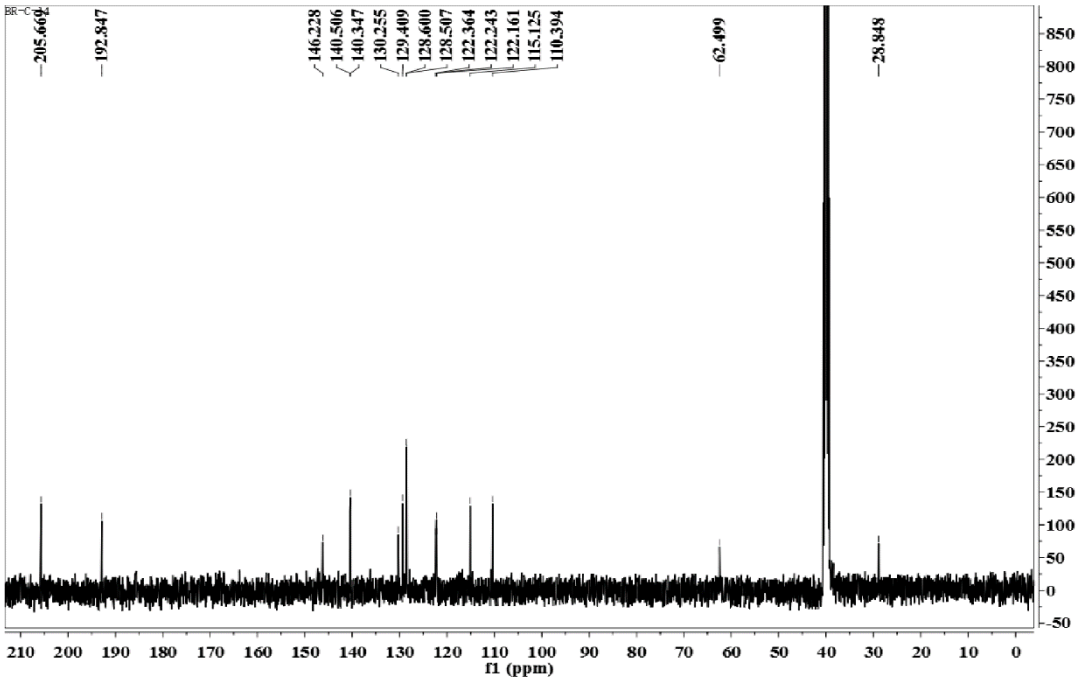
^{13}C NMR spectra of compound **5aaa**



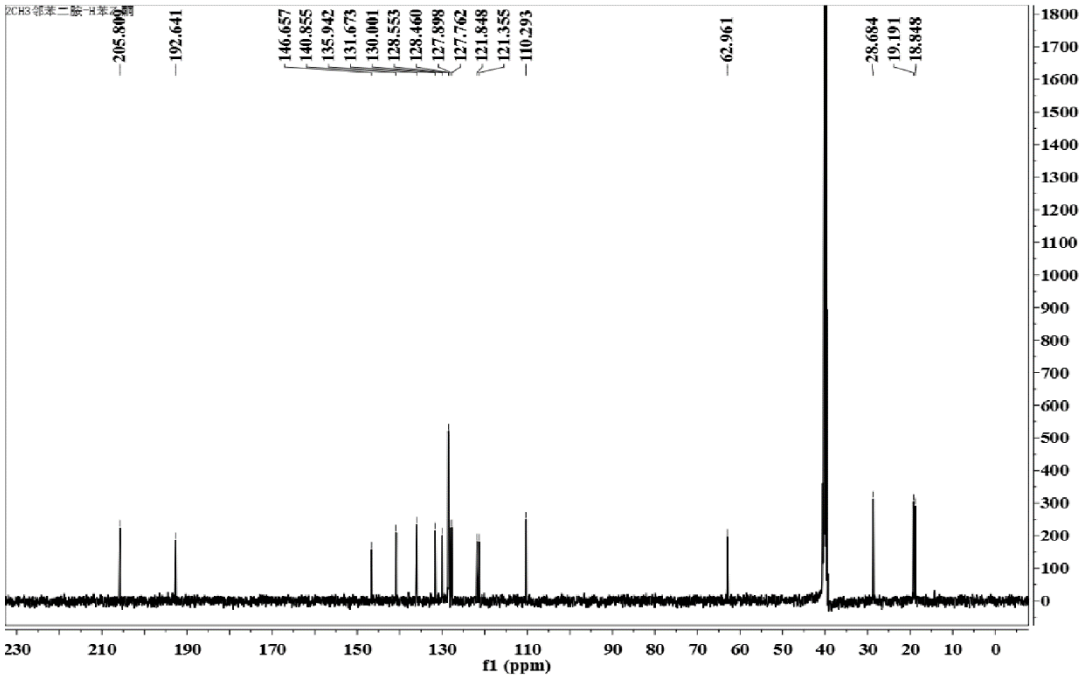
^{13}C NMR spectra of compound **5aba**



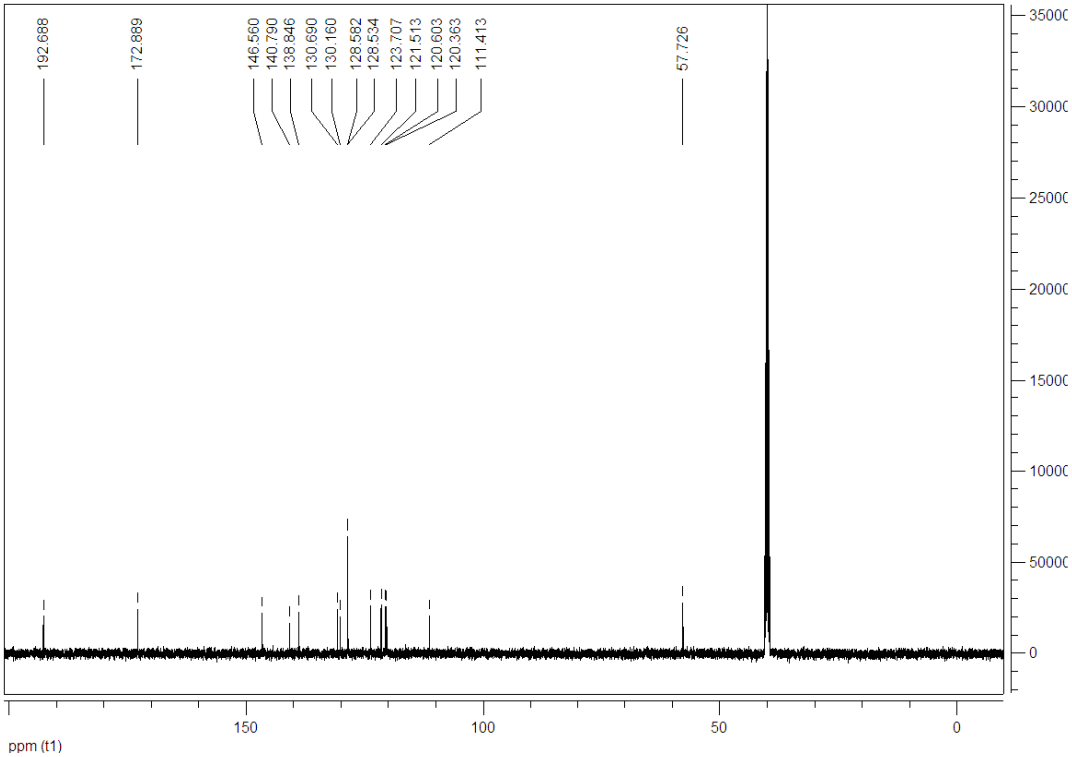
^{13}C NMR spectra of compound **5aca**



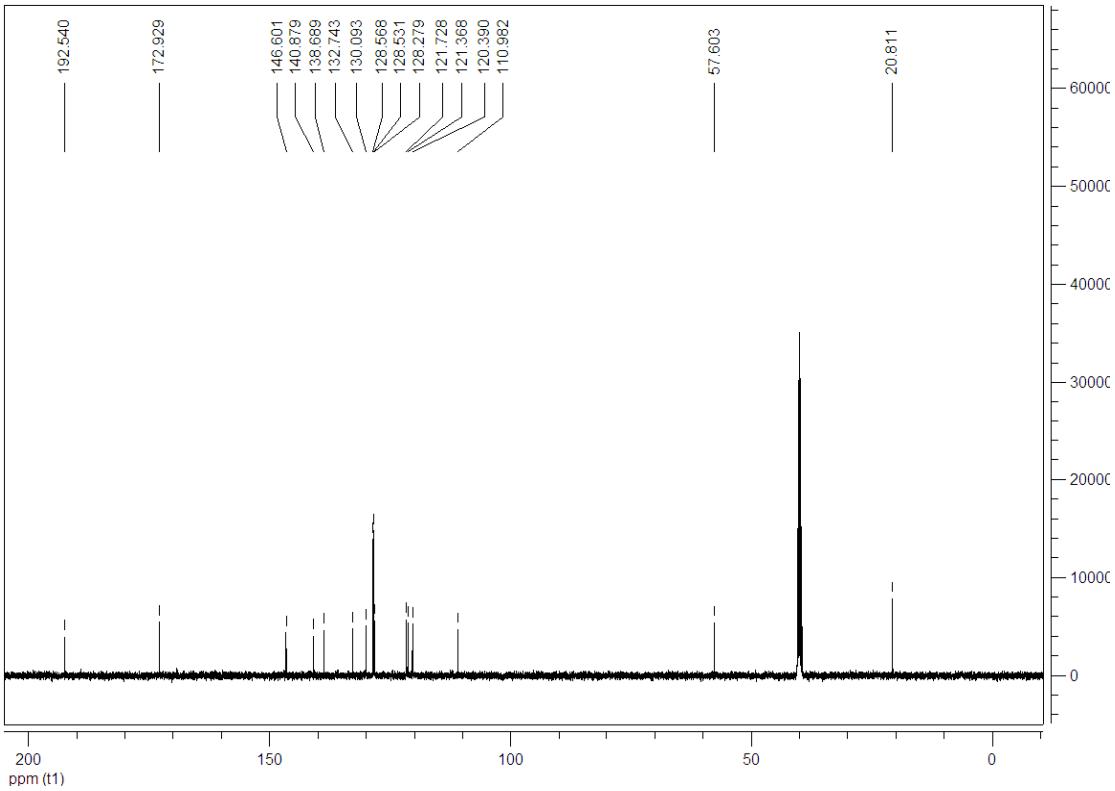
^{13}C NMR spectra of compound **5ada**



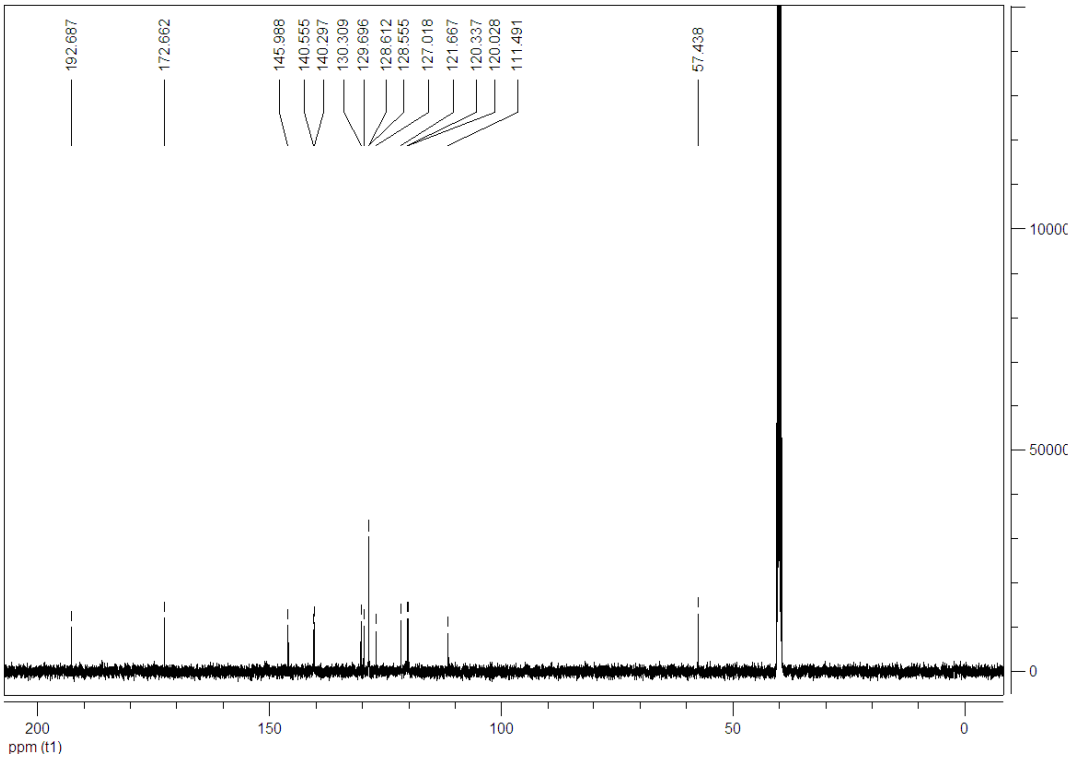
^{13}C NMR spectra of compound **5aea**



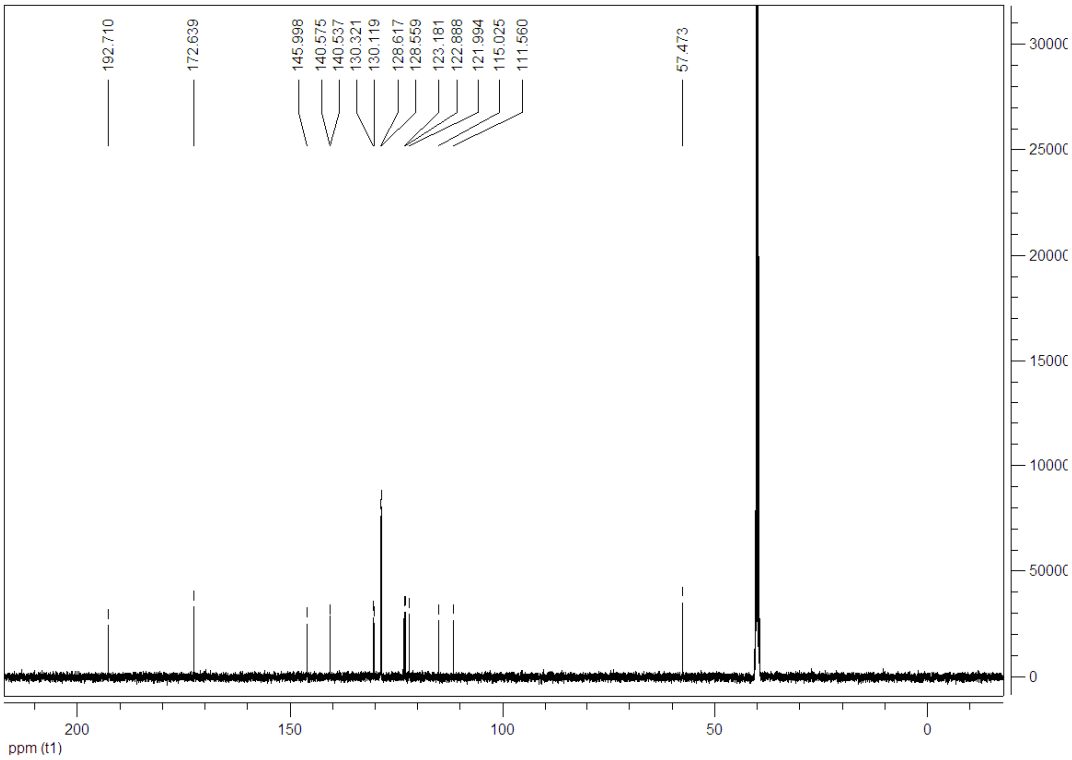
^{13}C NMR spectra of compound **5aab**



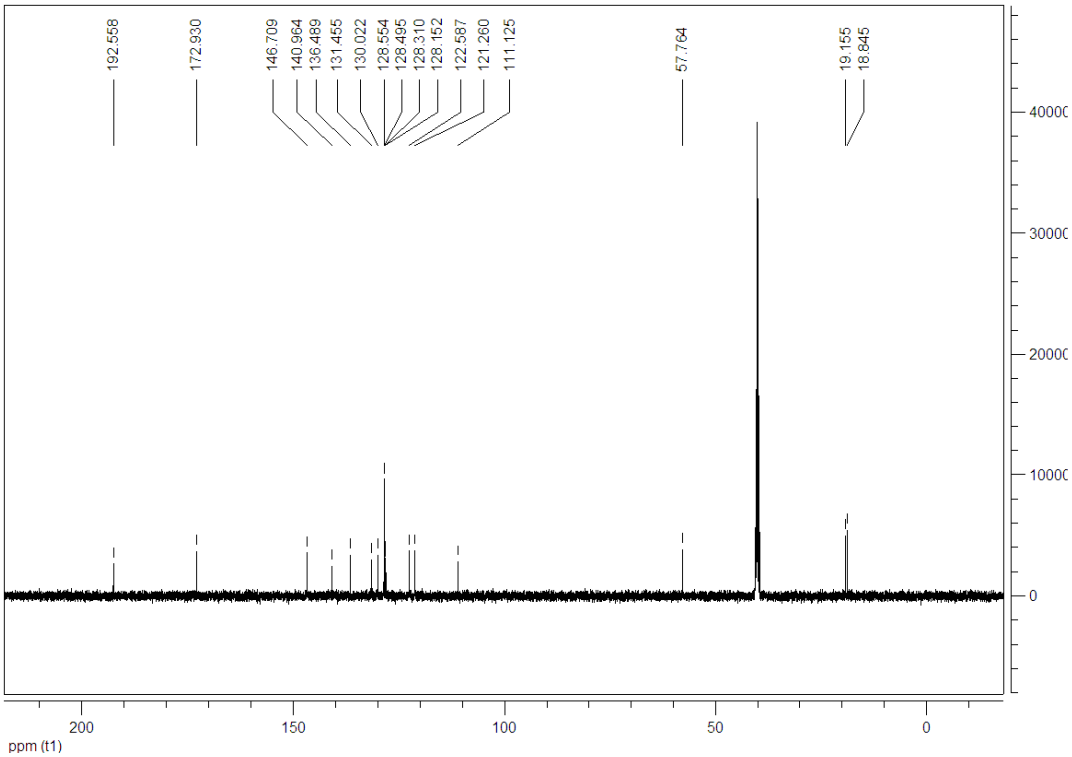
^{13}C NMR spectra of compound **5abb**



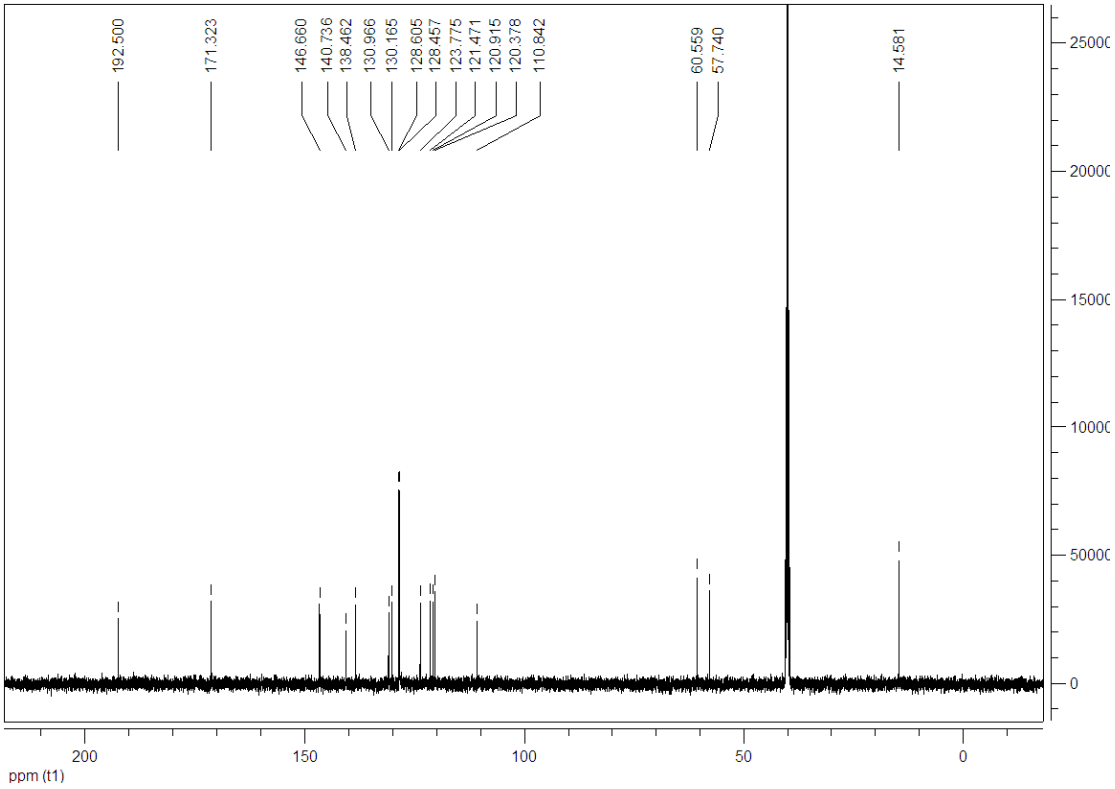
^{13}C NMR spectra of compound **5acb**



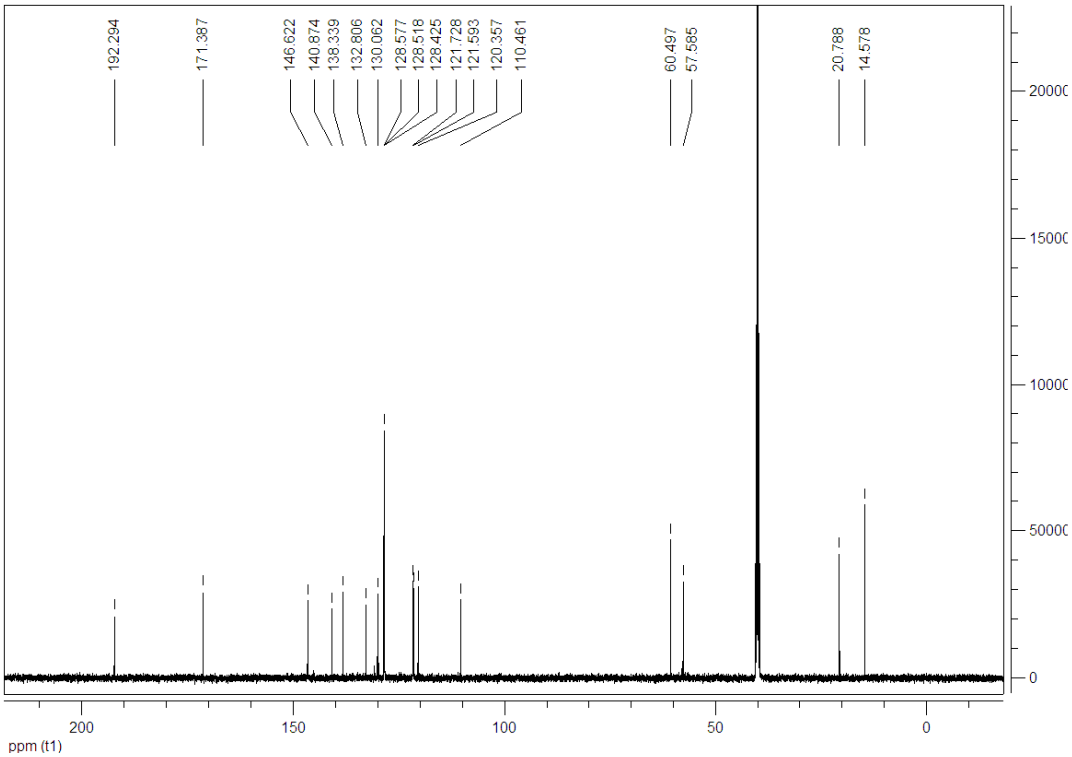
^{13}C NMR spectra of compound **5adb**



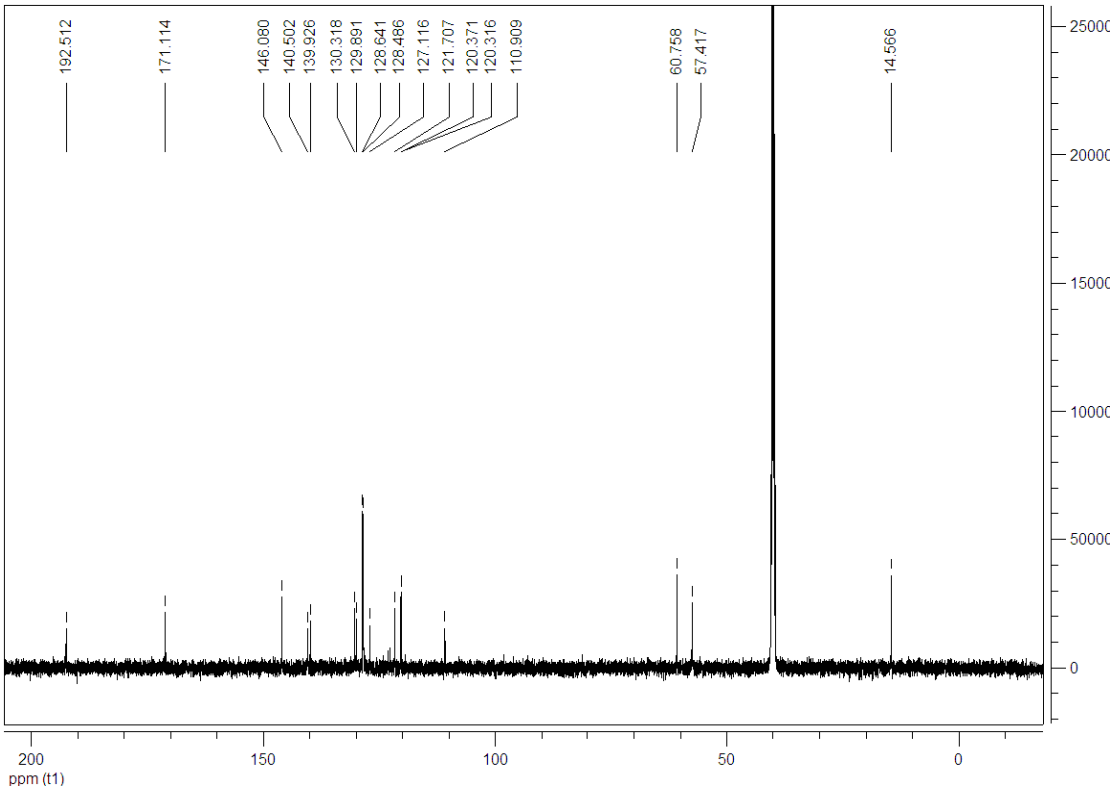
^{13}C NMR spectra of compound **5aeb**



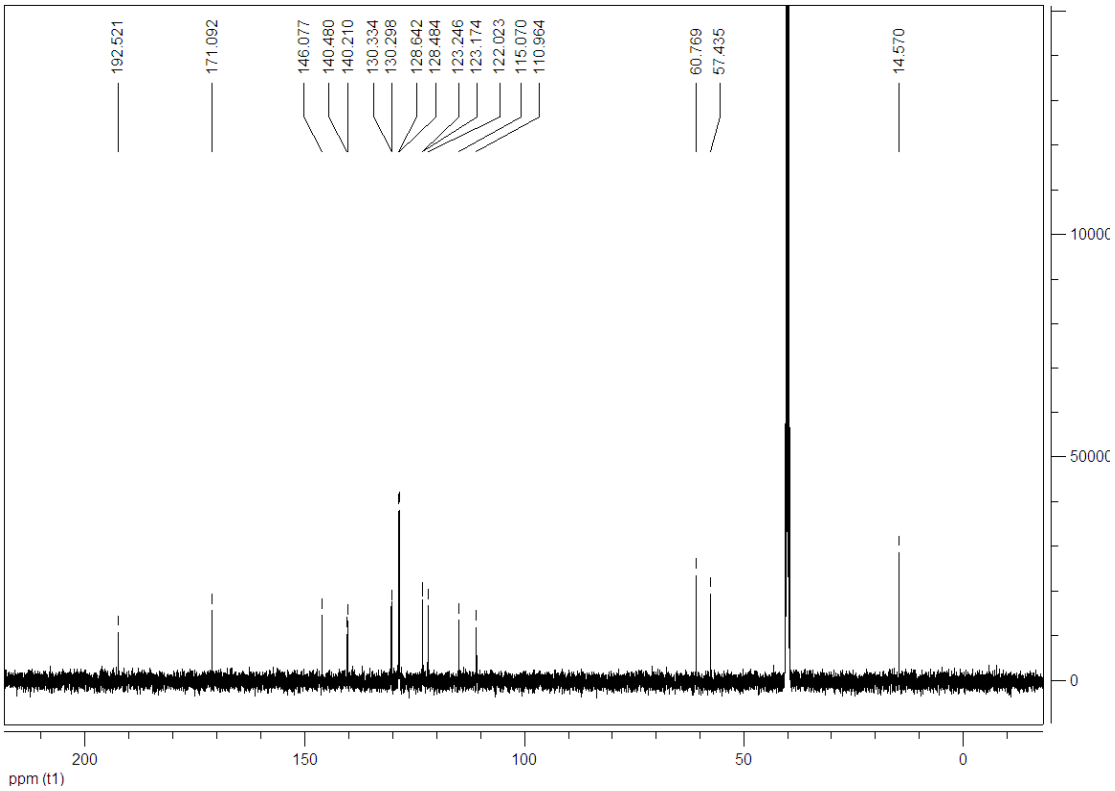
^{13}C NMR spectra of compound **5aac**



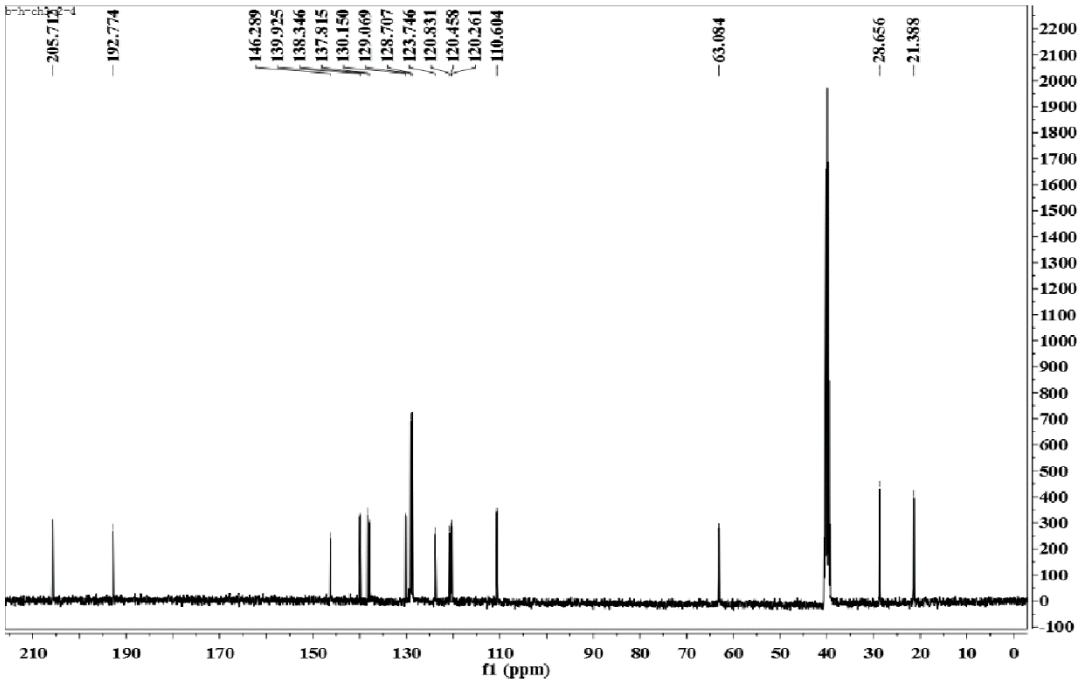
^{13}C NMR spectra of compound **5abc**



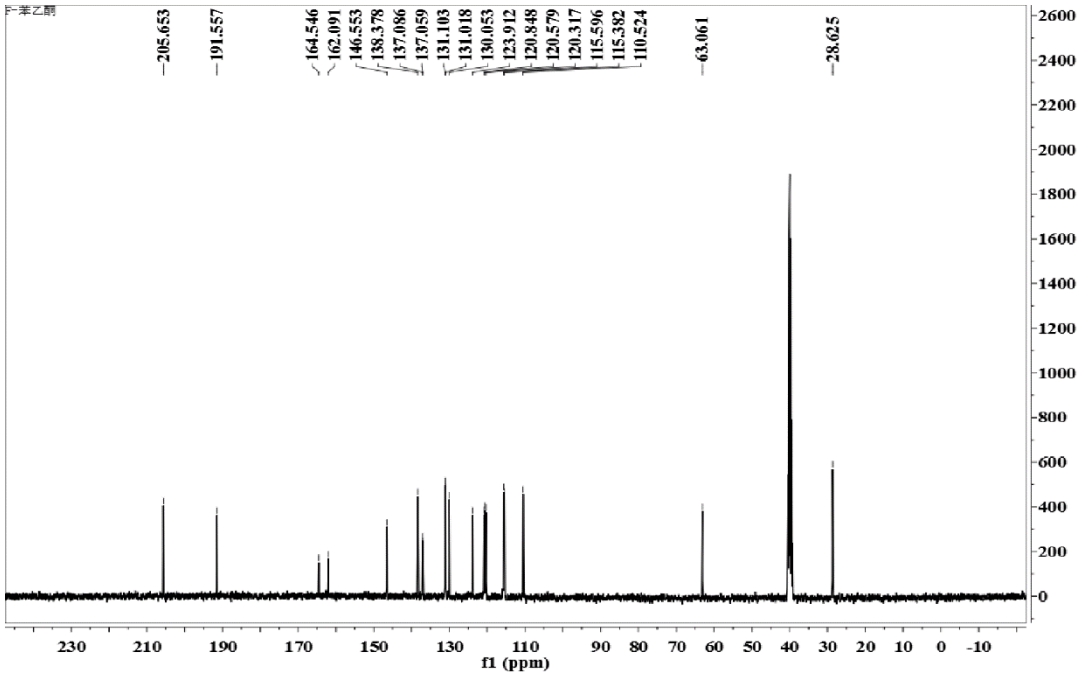
^{13}C NMR spectra of compound **5acc**



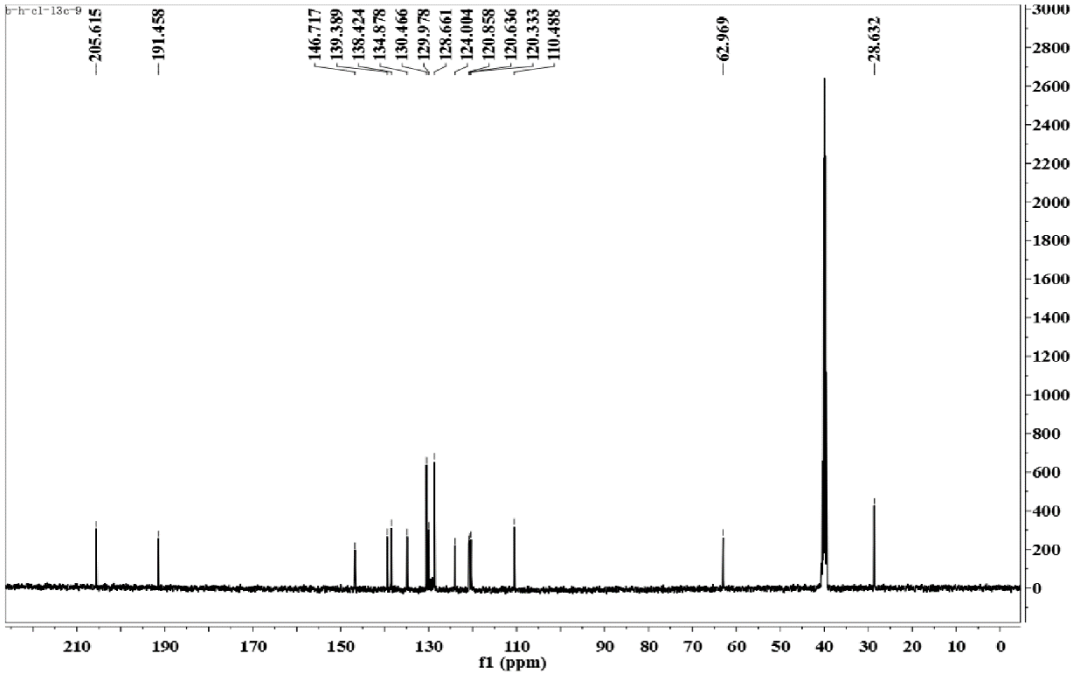
^{13}C NMR spectra of compound **5adc**



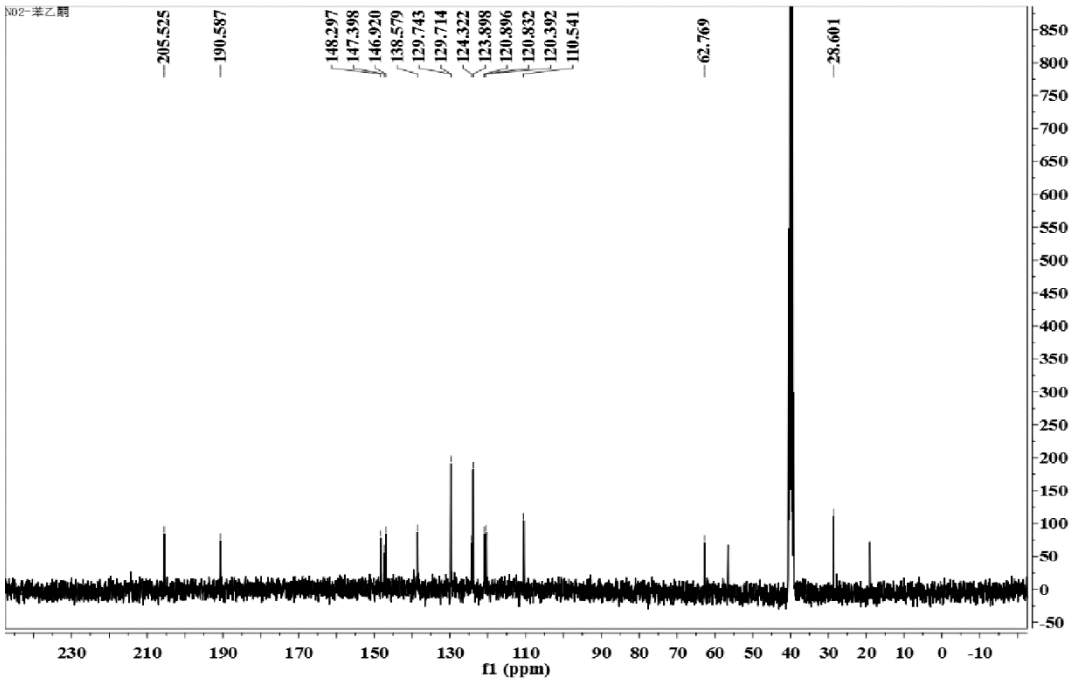
^{13}C NMR spectra of compound **5baa**



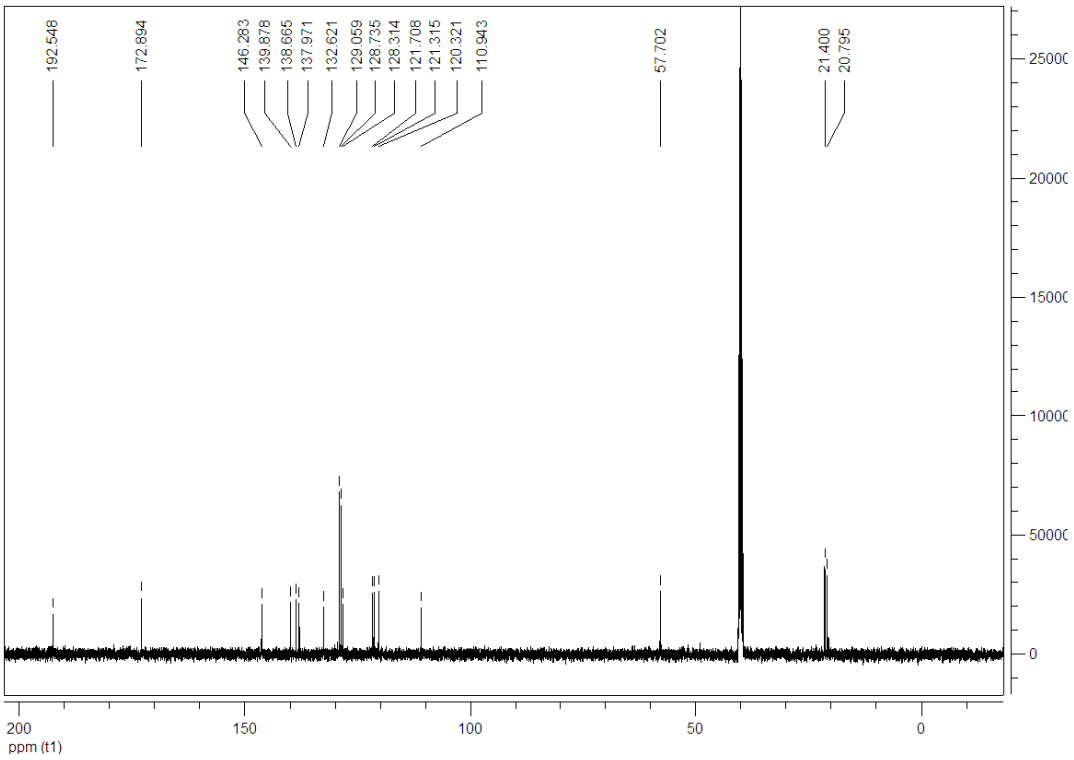
^{13}C NMR spectra of compound **5caa**



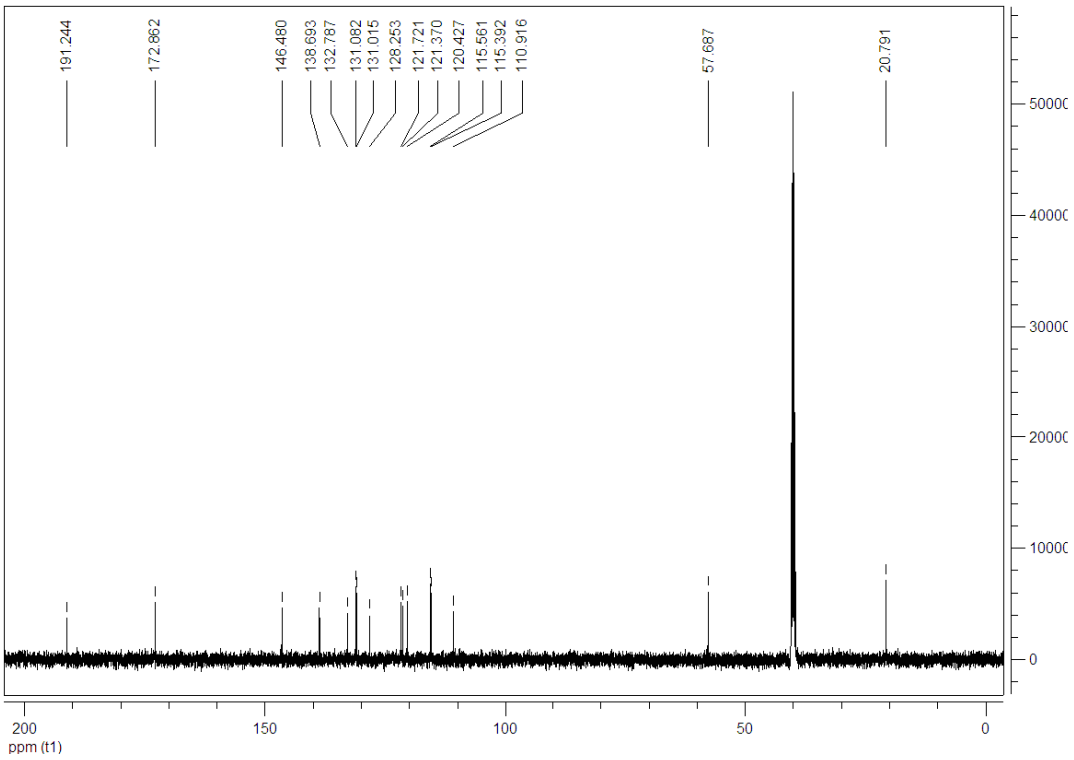
^{13}C NMR spectra of compound **5daa**



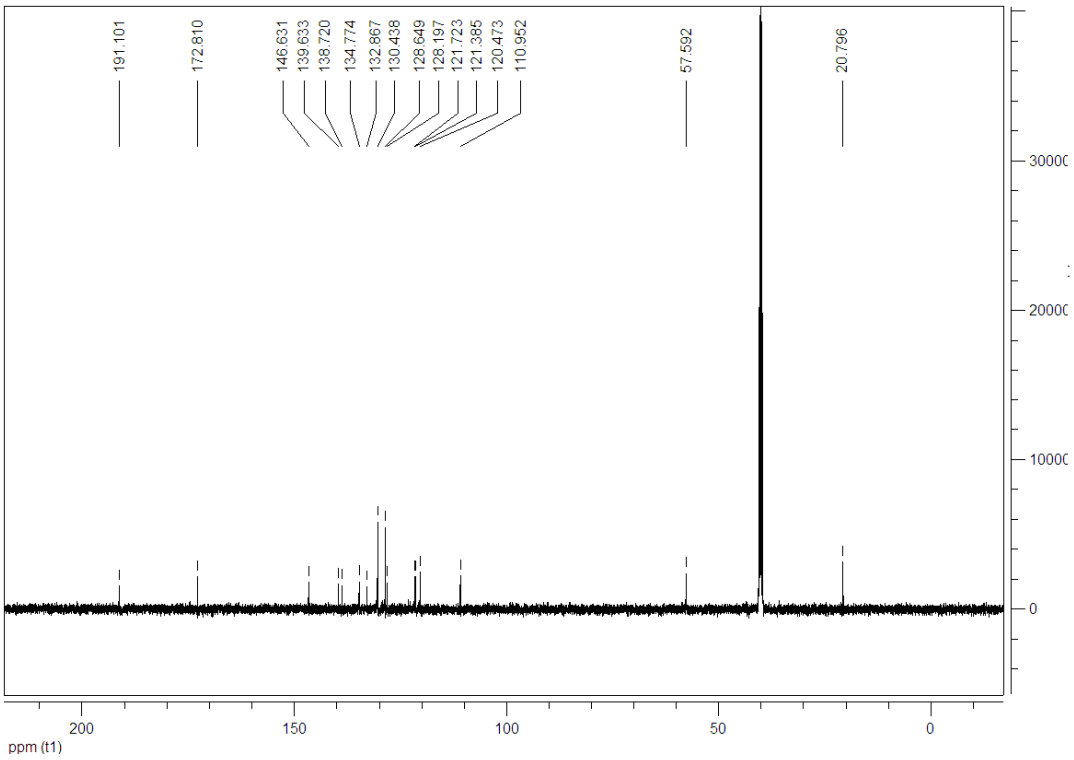
^{13}C NMR spectra of compound **5eaa**



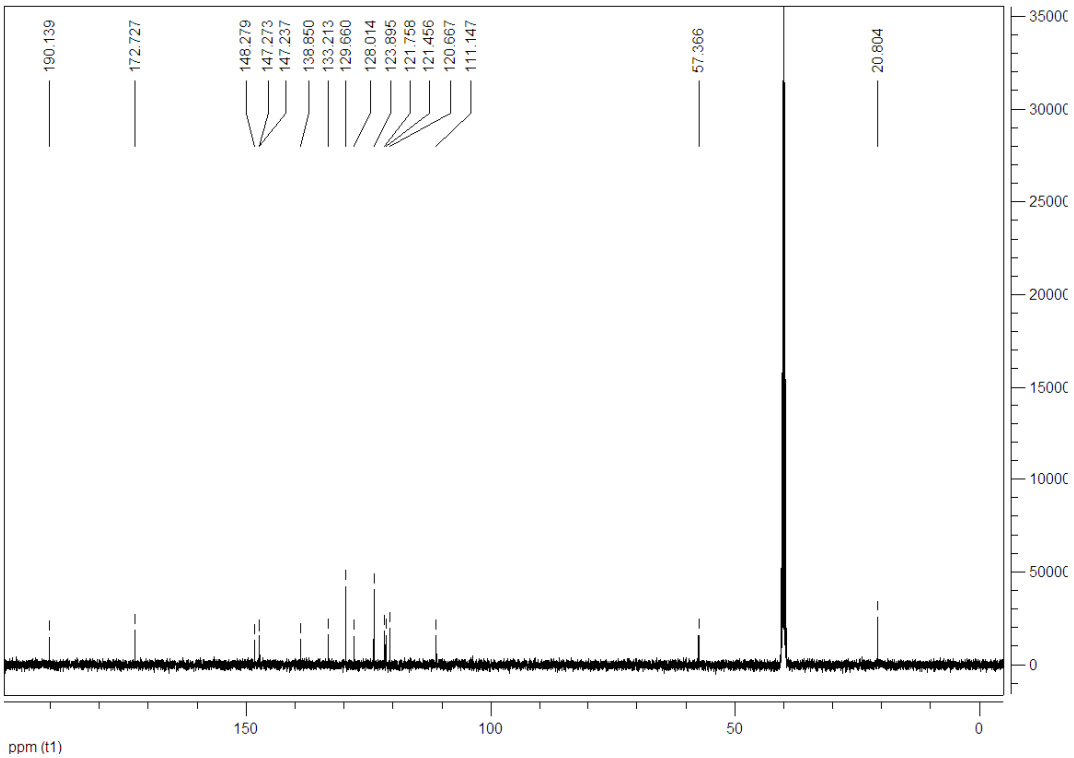
^{13}C NMR spectra of compound **5bbb**



^{13}C NMR spectra of compound **5cbb**



^{13}C NMR spectra of compound **5dbb**



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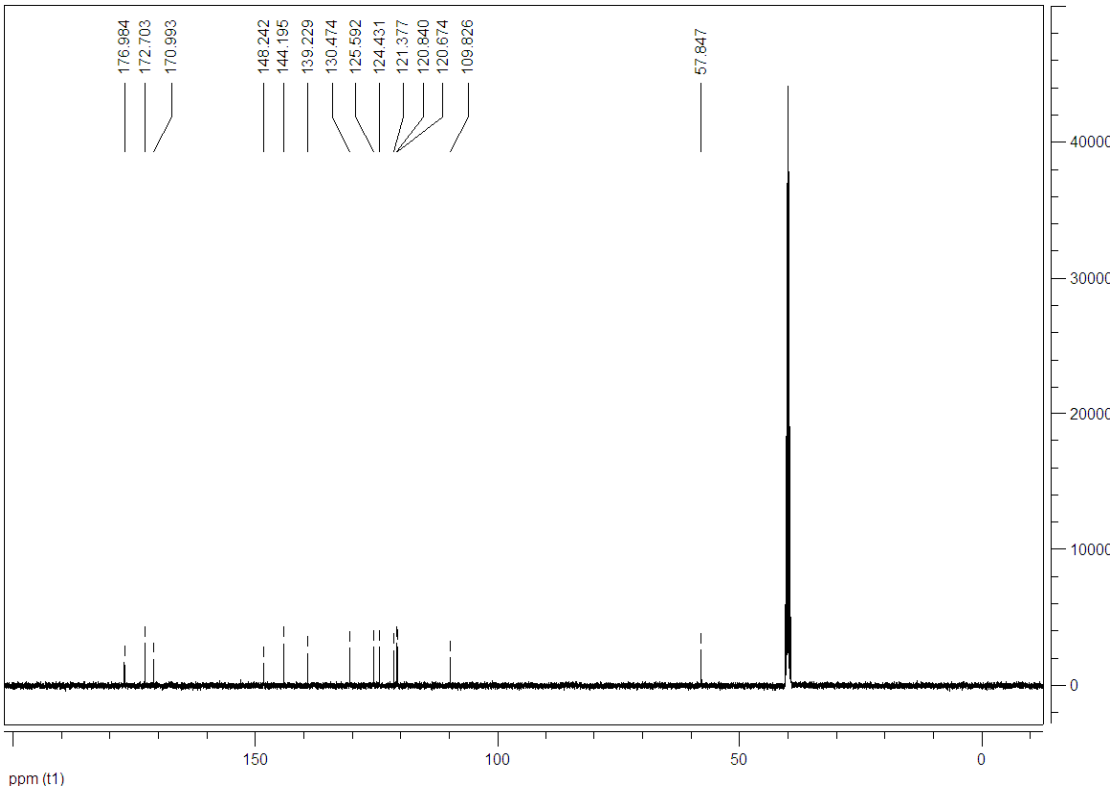
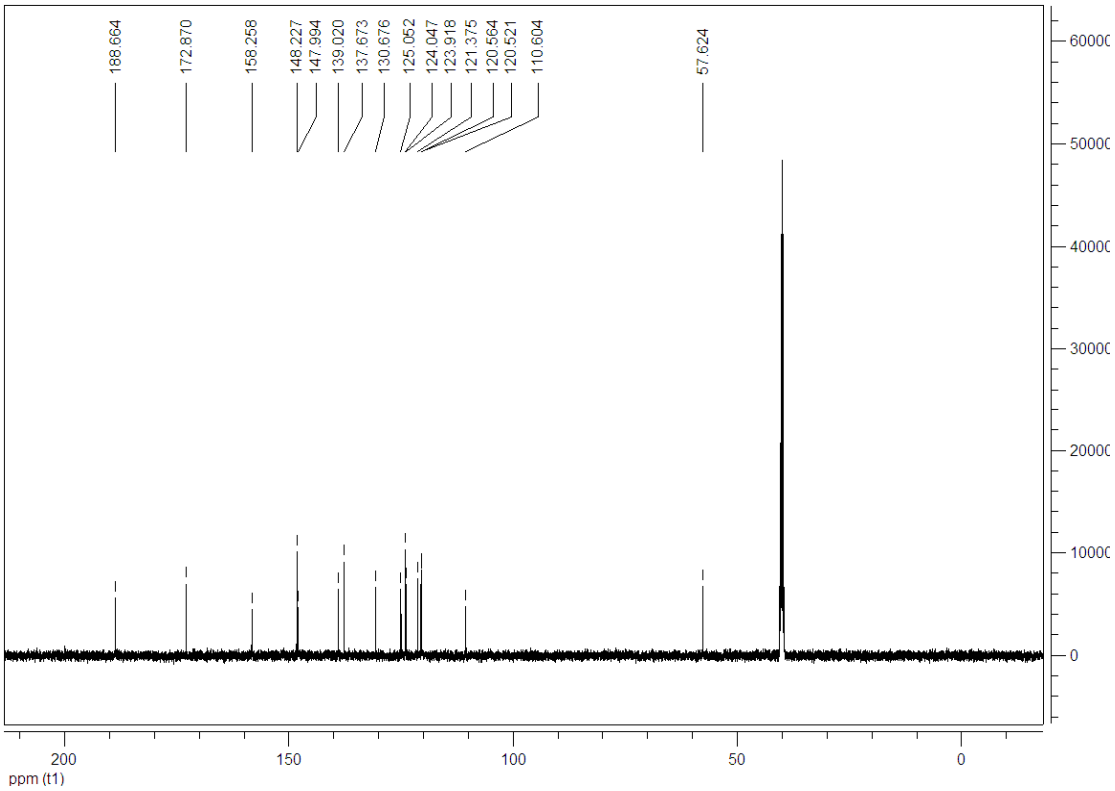


^{13}C NMR spectra of compound **5fab**



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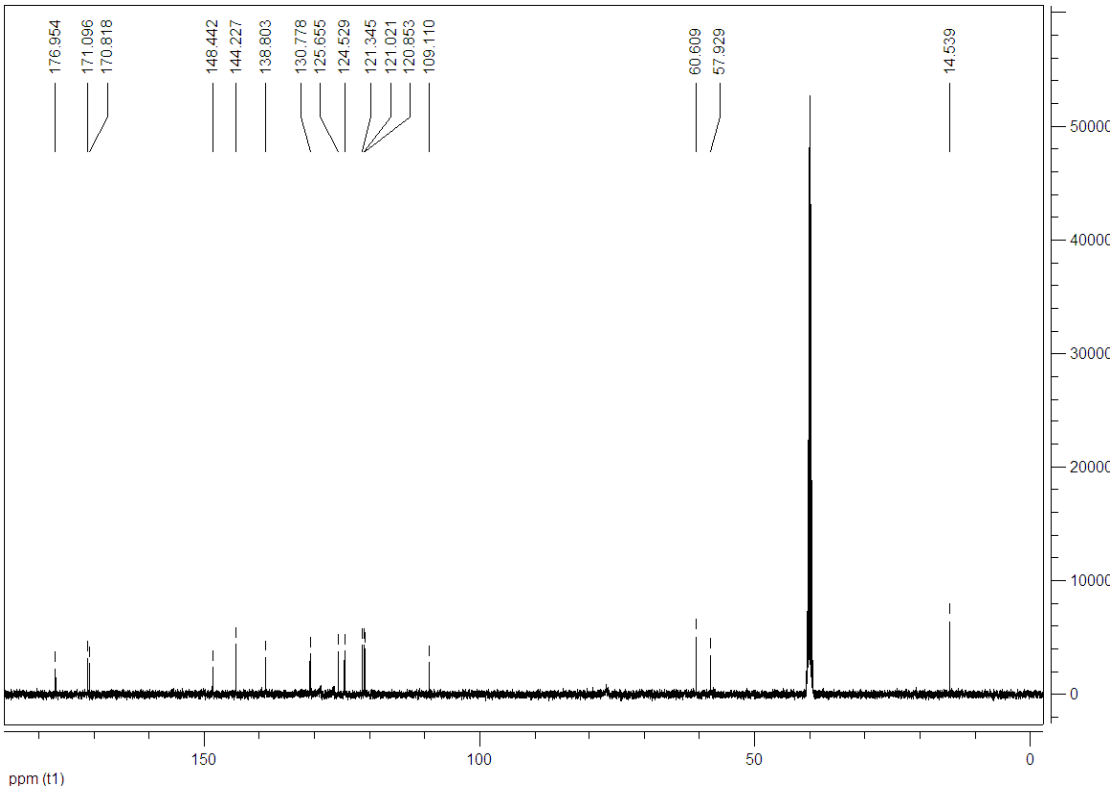
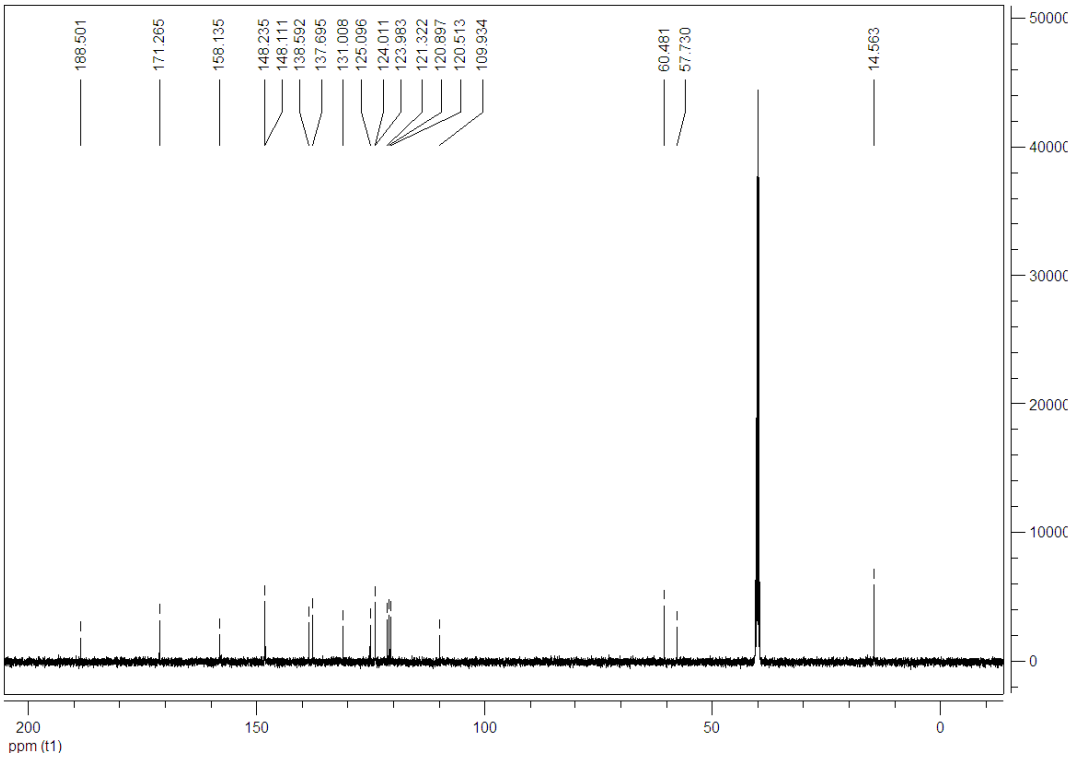
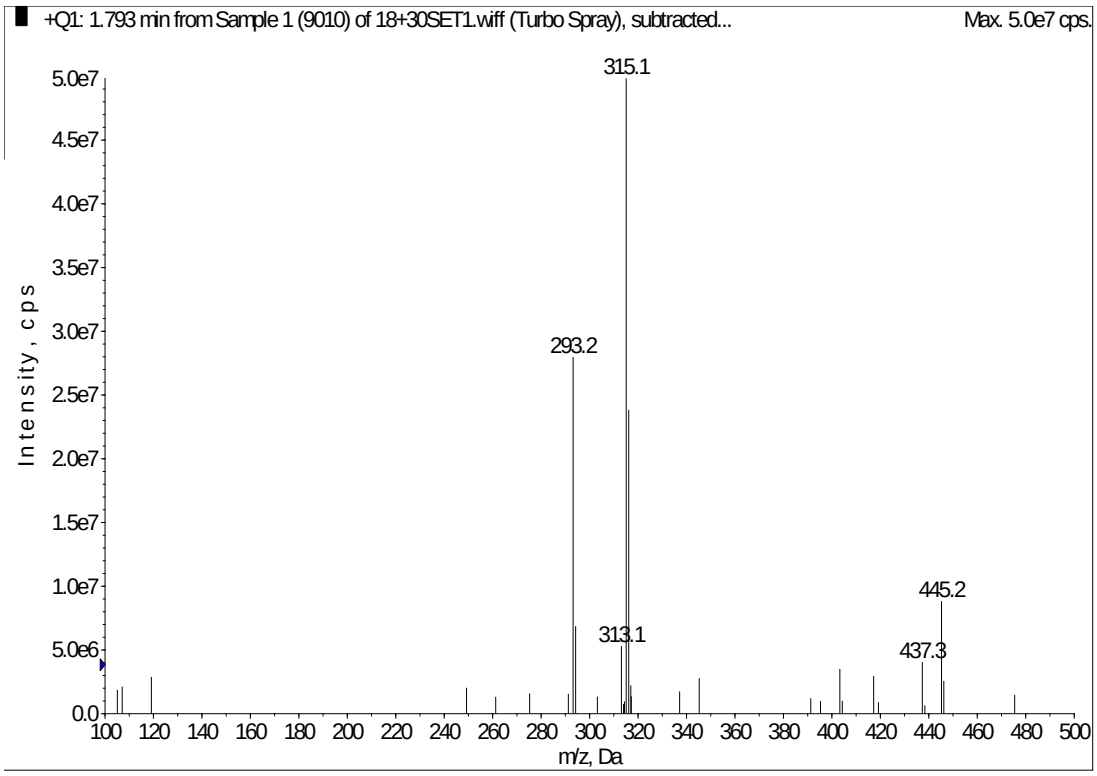


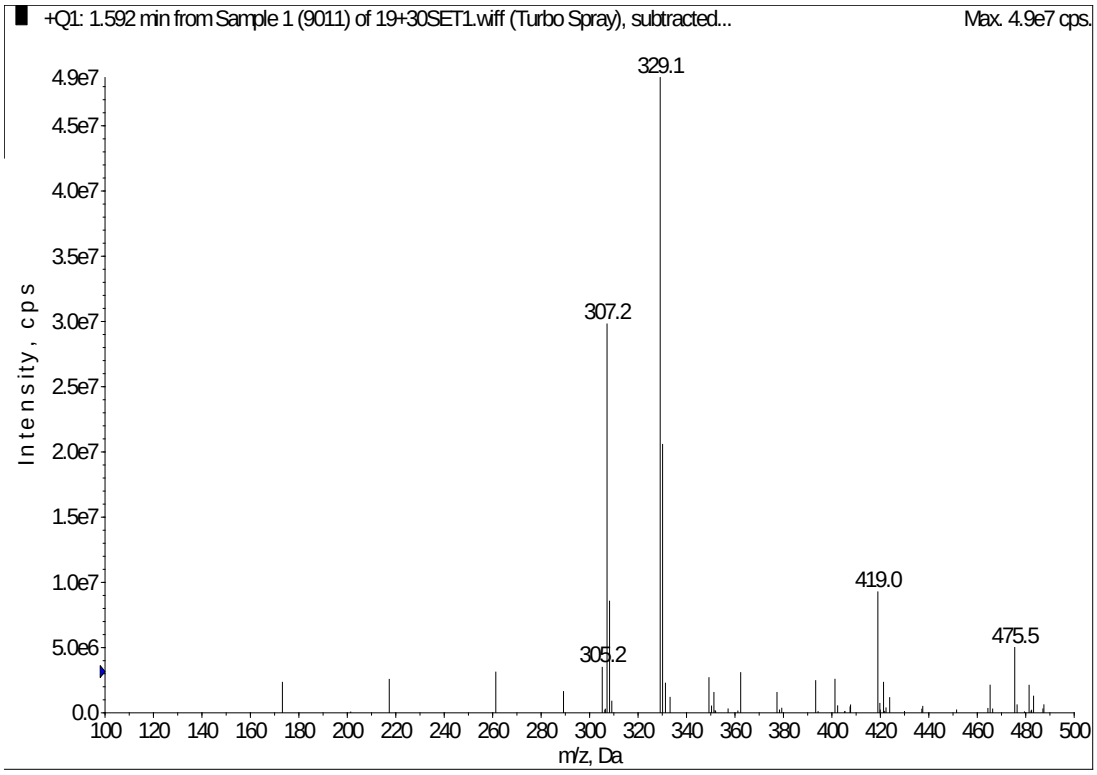
^{13}C NMR spectra of compound **5fac**



^{13}C NMR spectra of compound **5gac**



MS of compound **5aaa**



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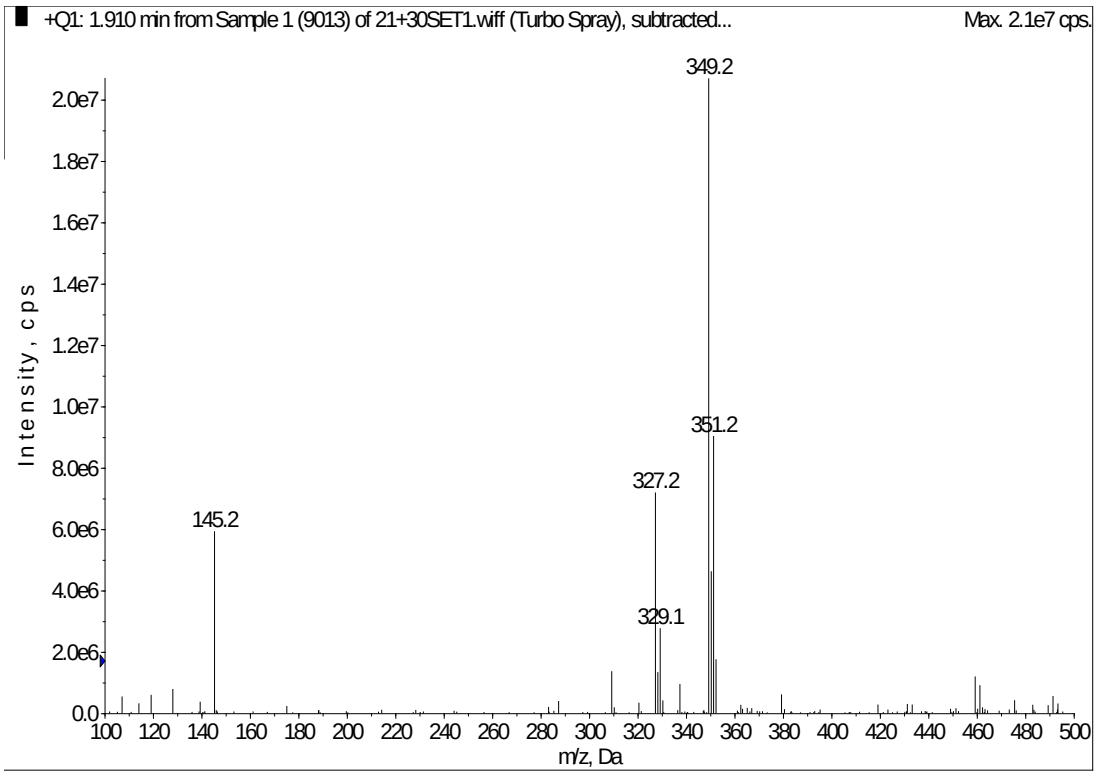

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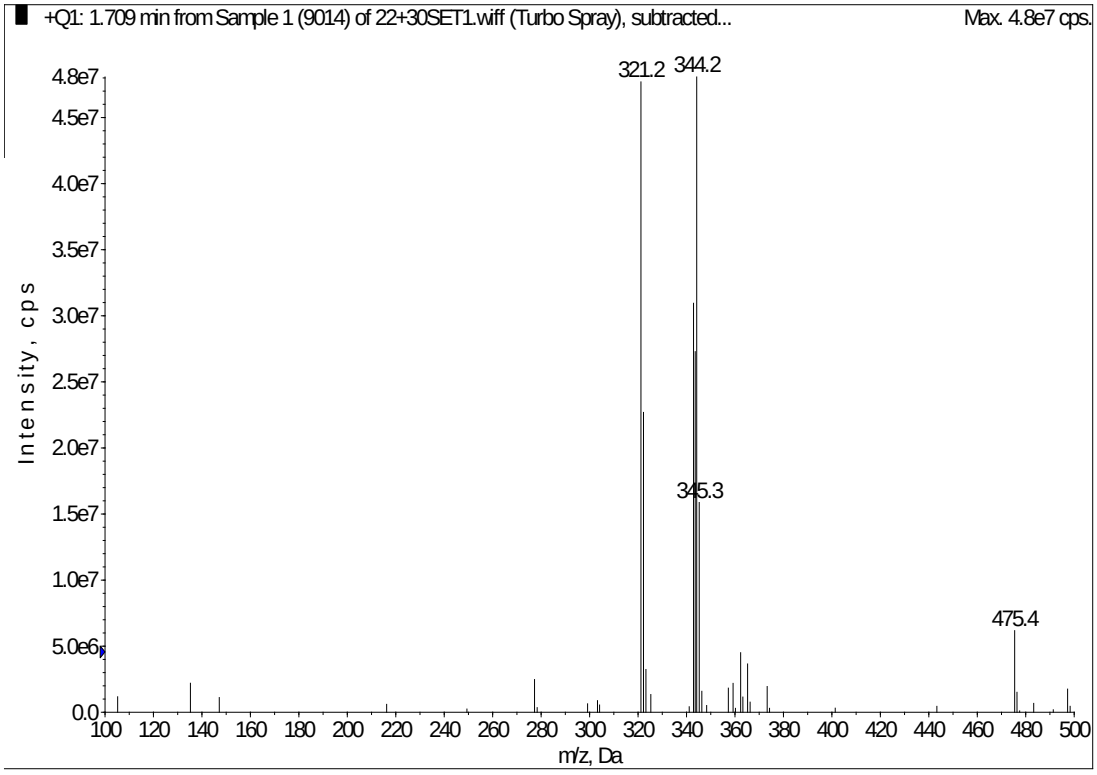

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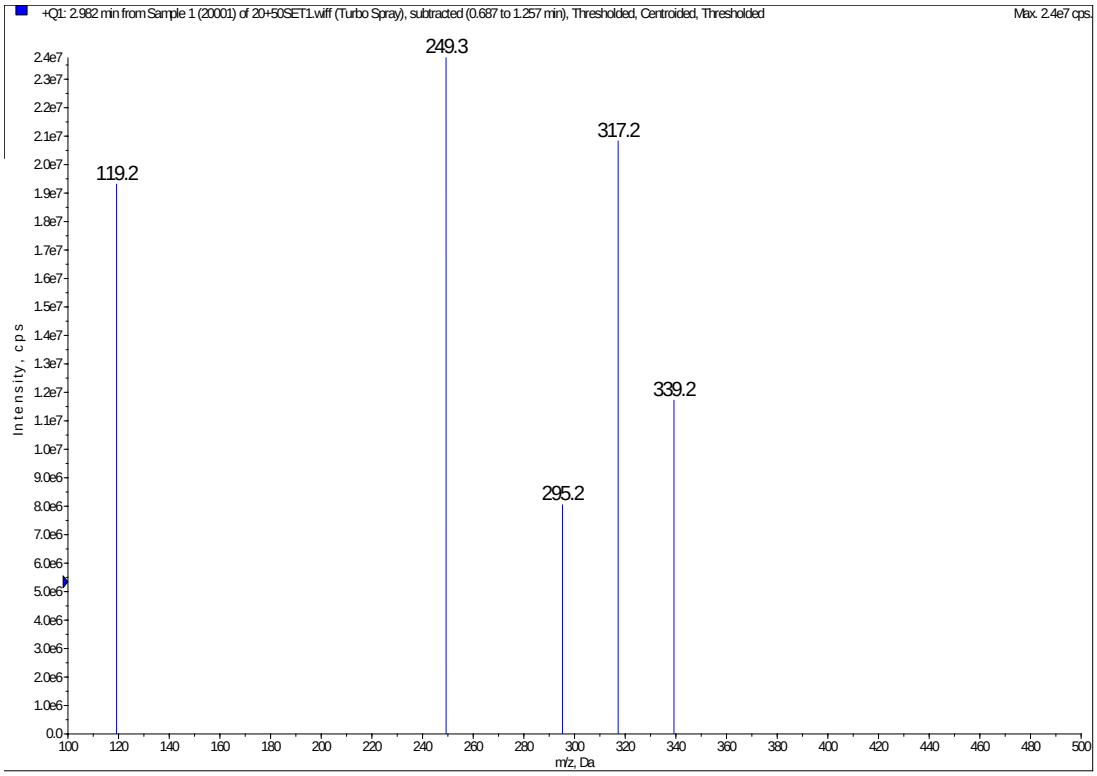

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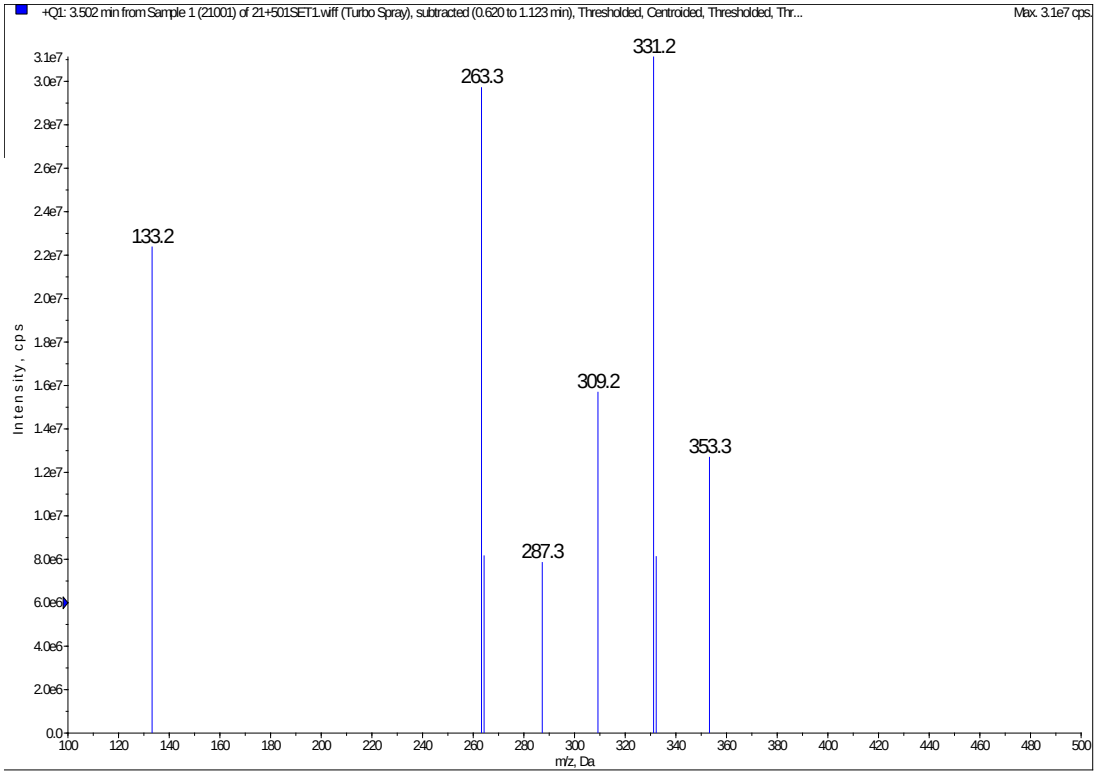

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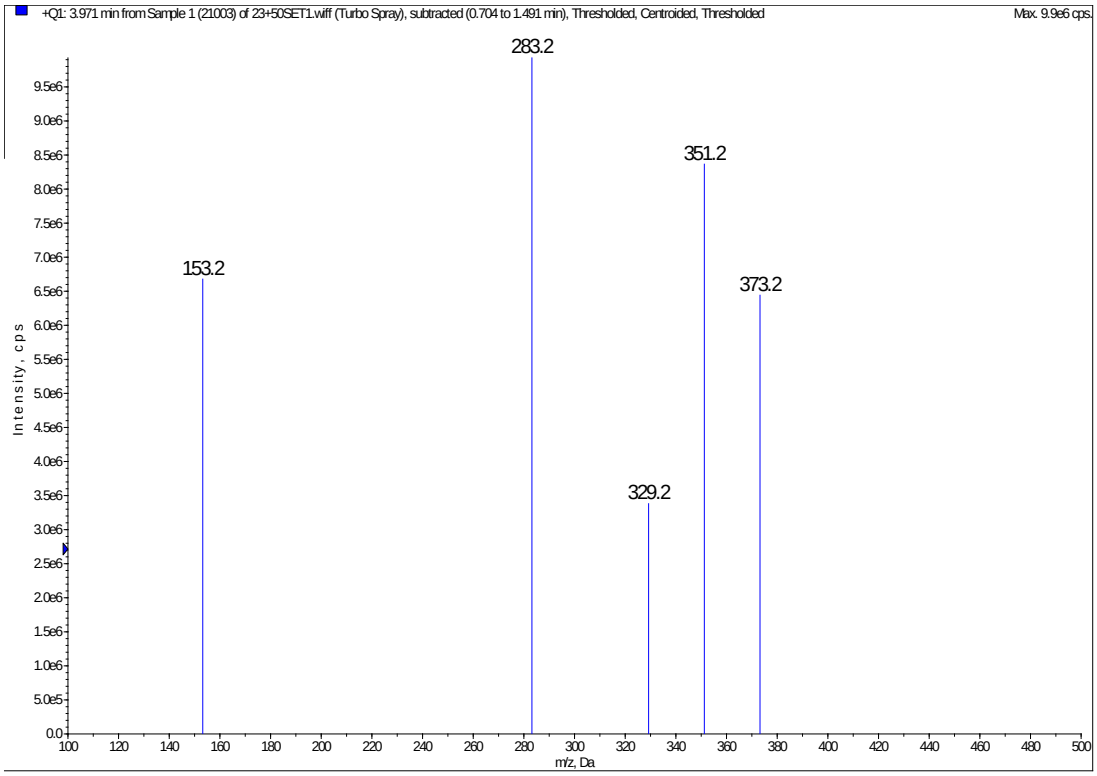
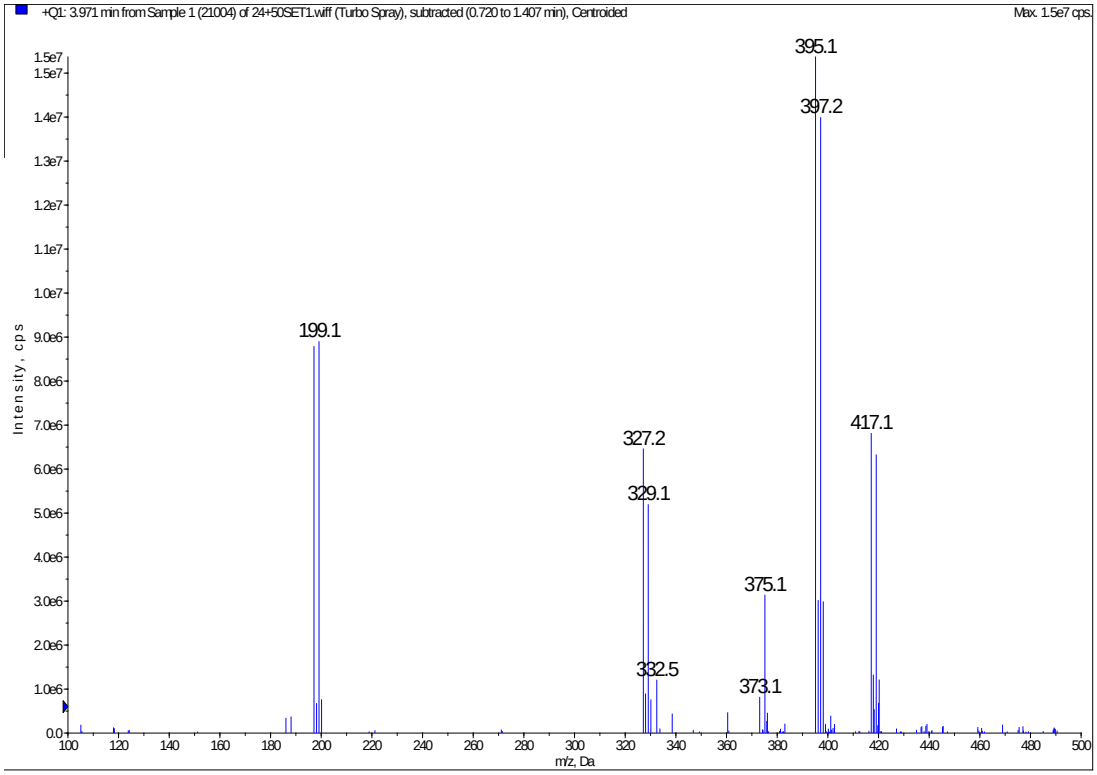
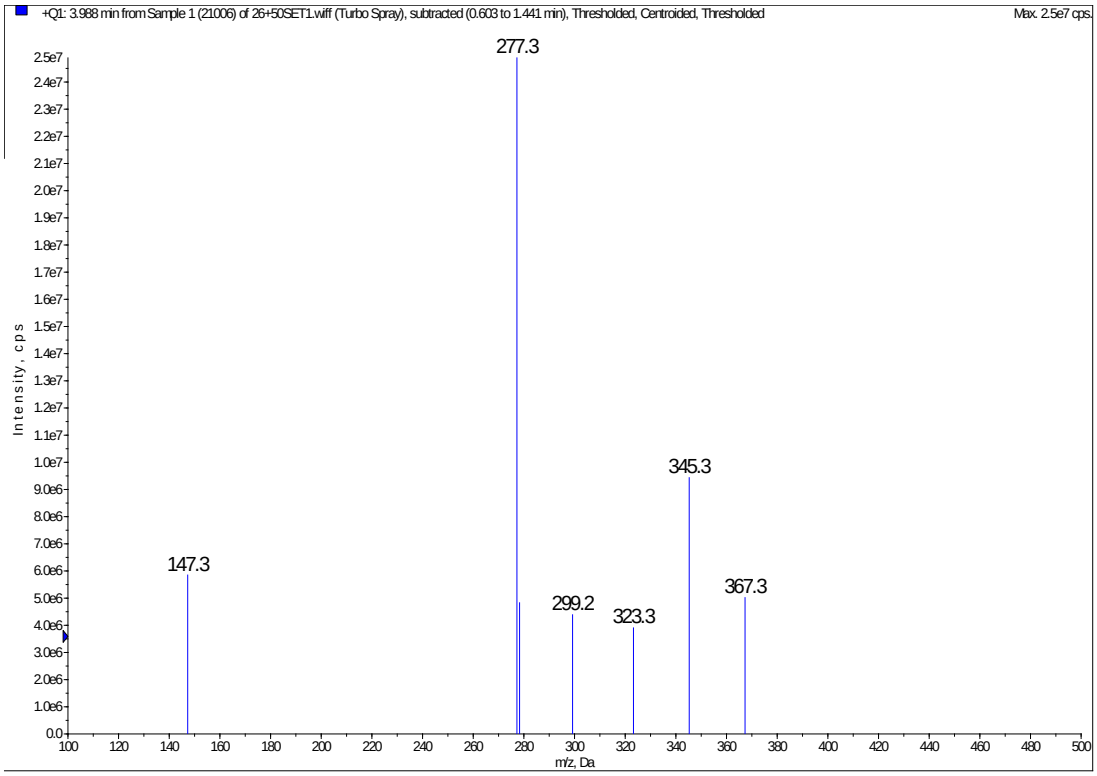


MS of compound **5acb**



MS of compound **5adb**



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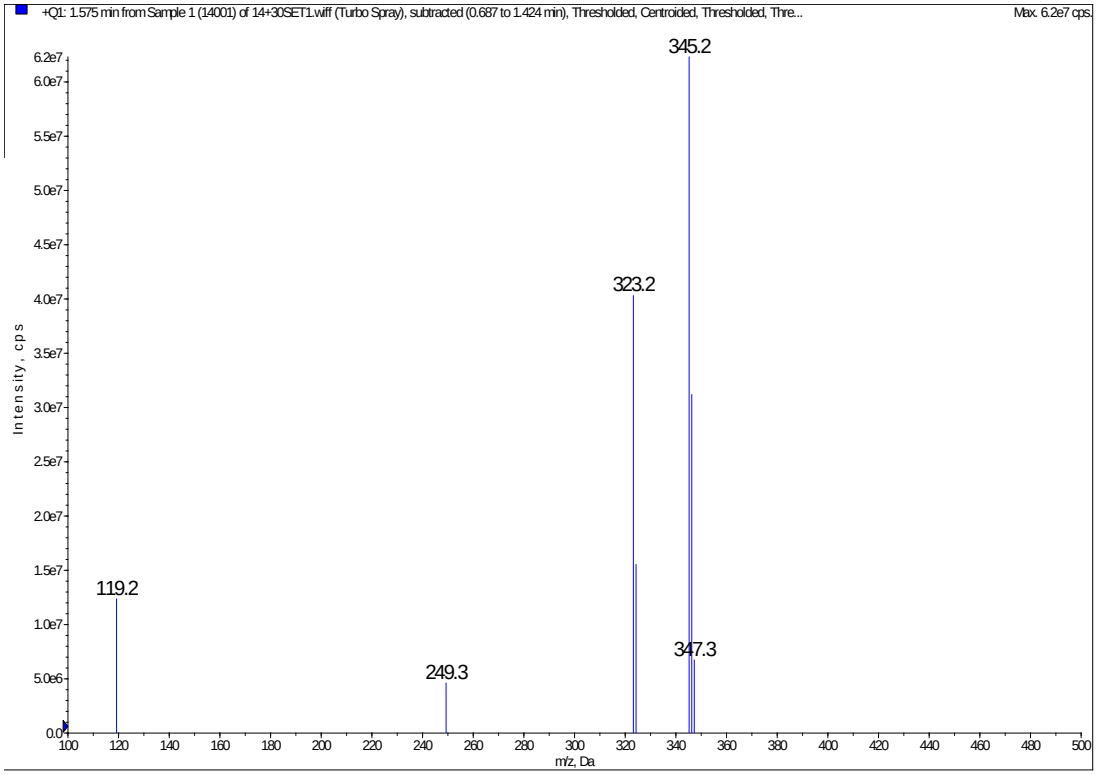

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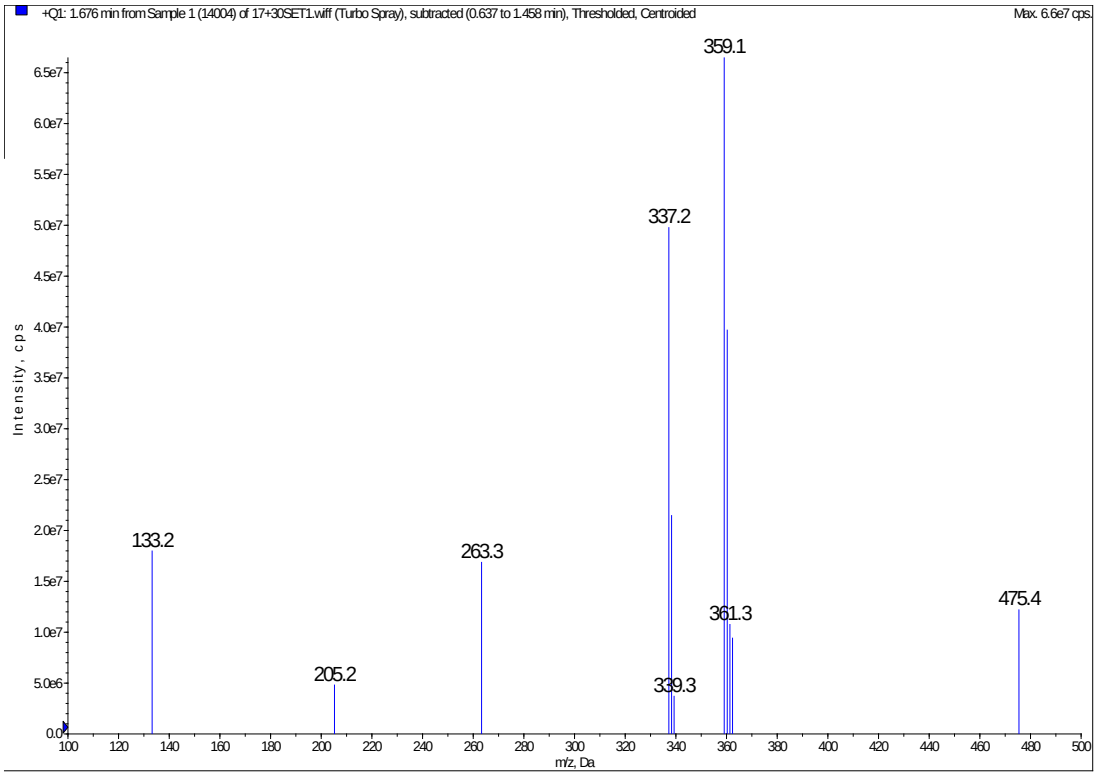
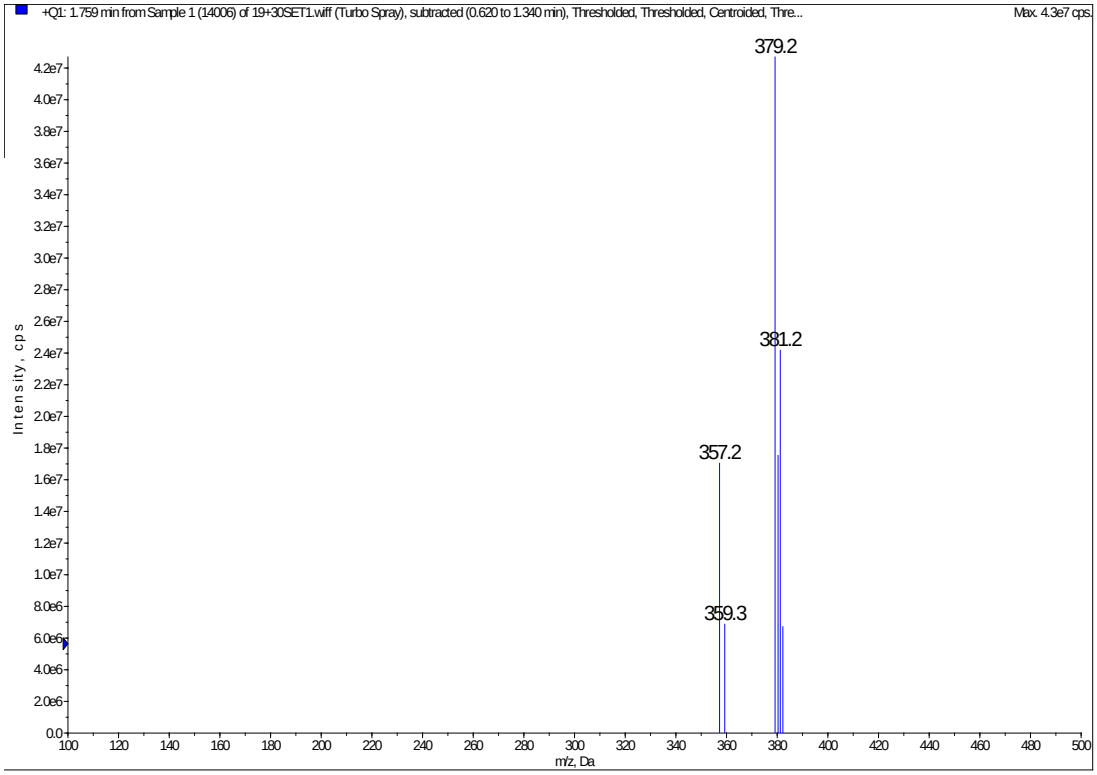


MS of compound **5abc**



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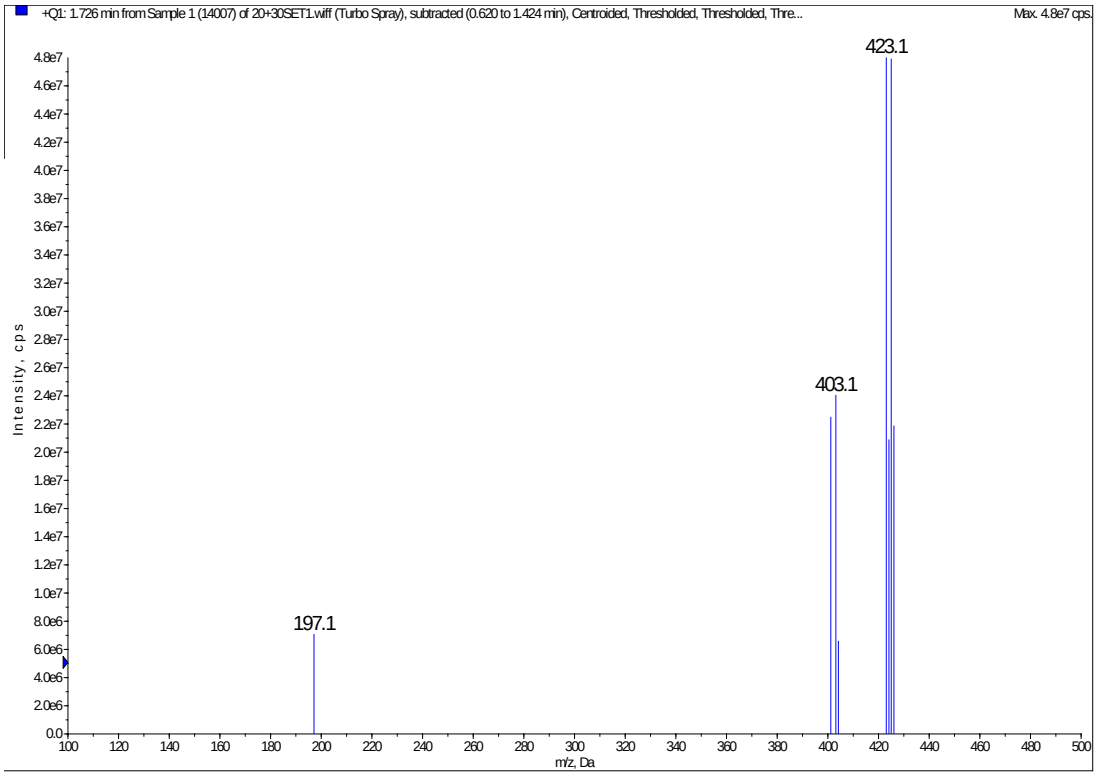

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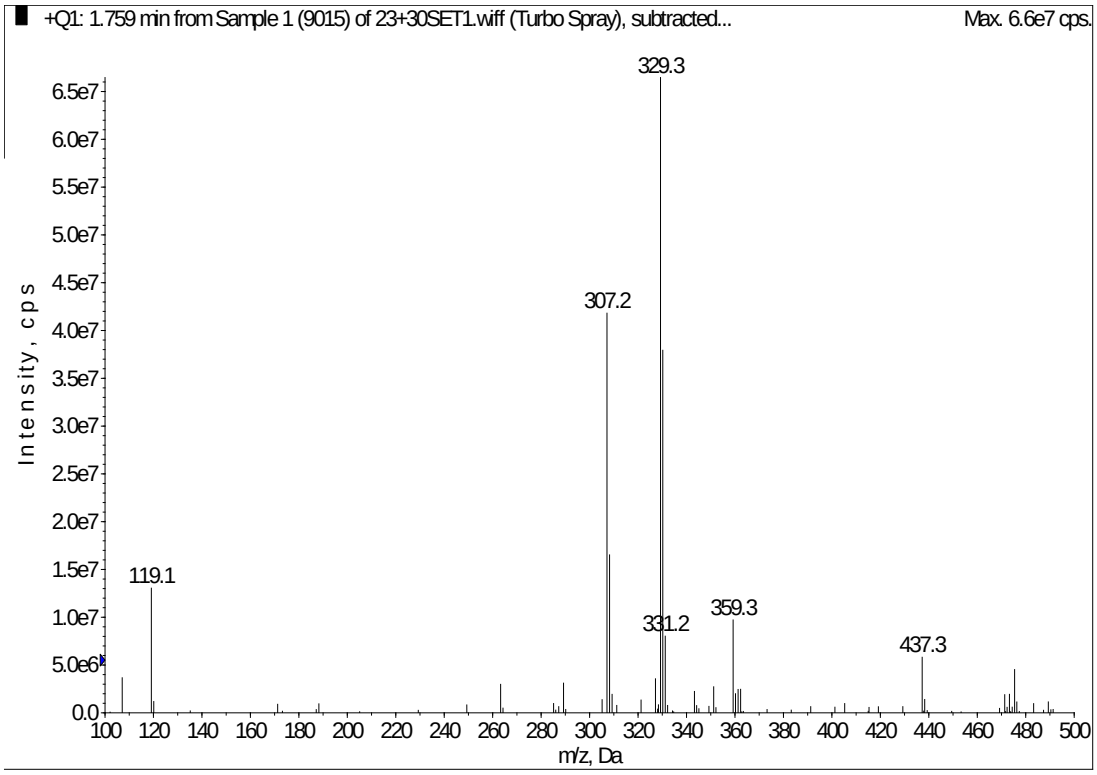

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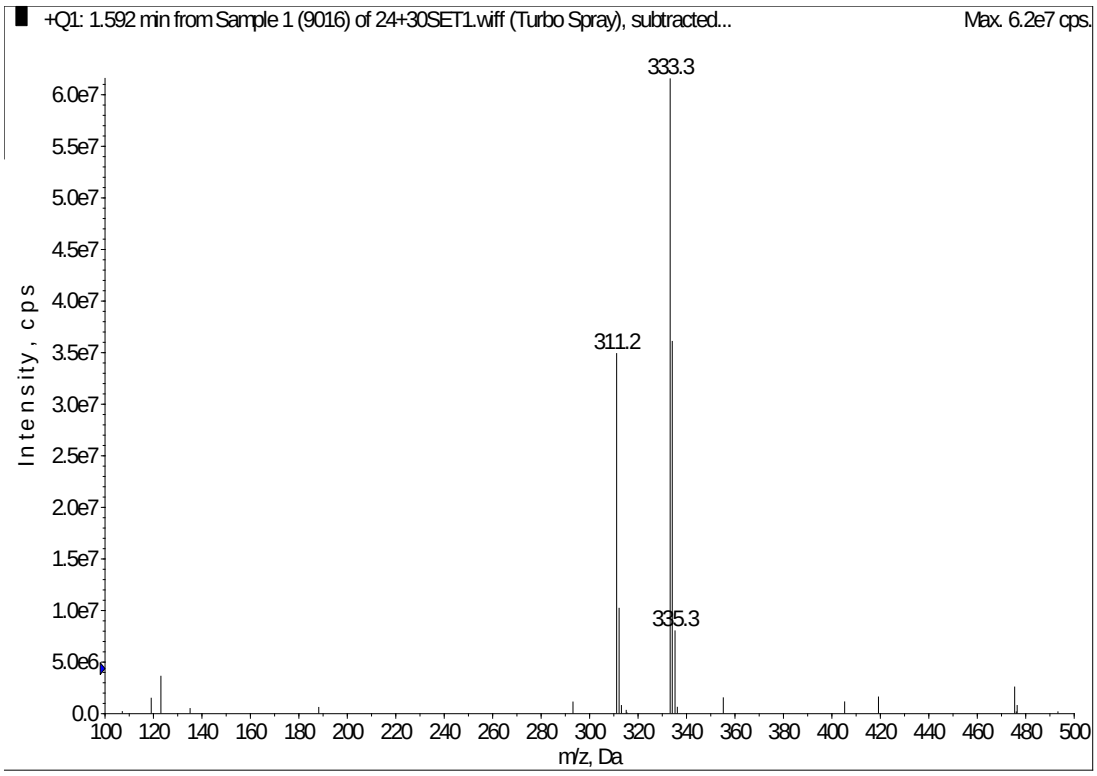

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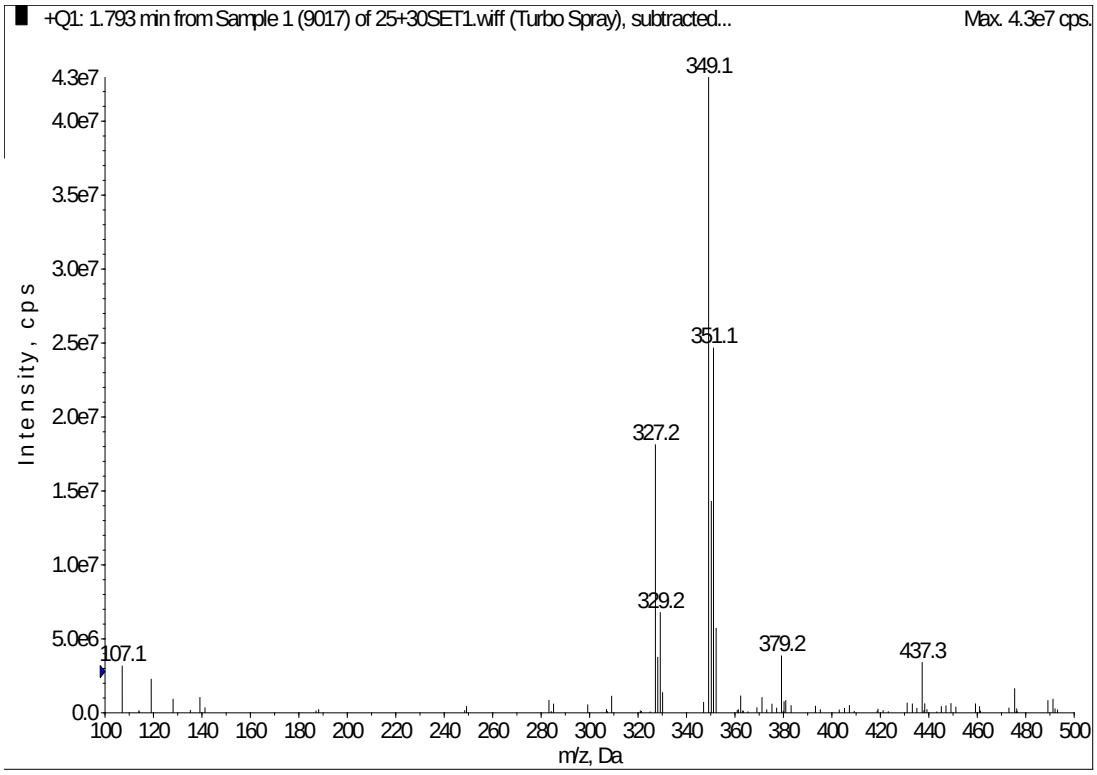
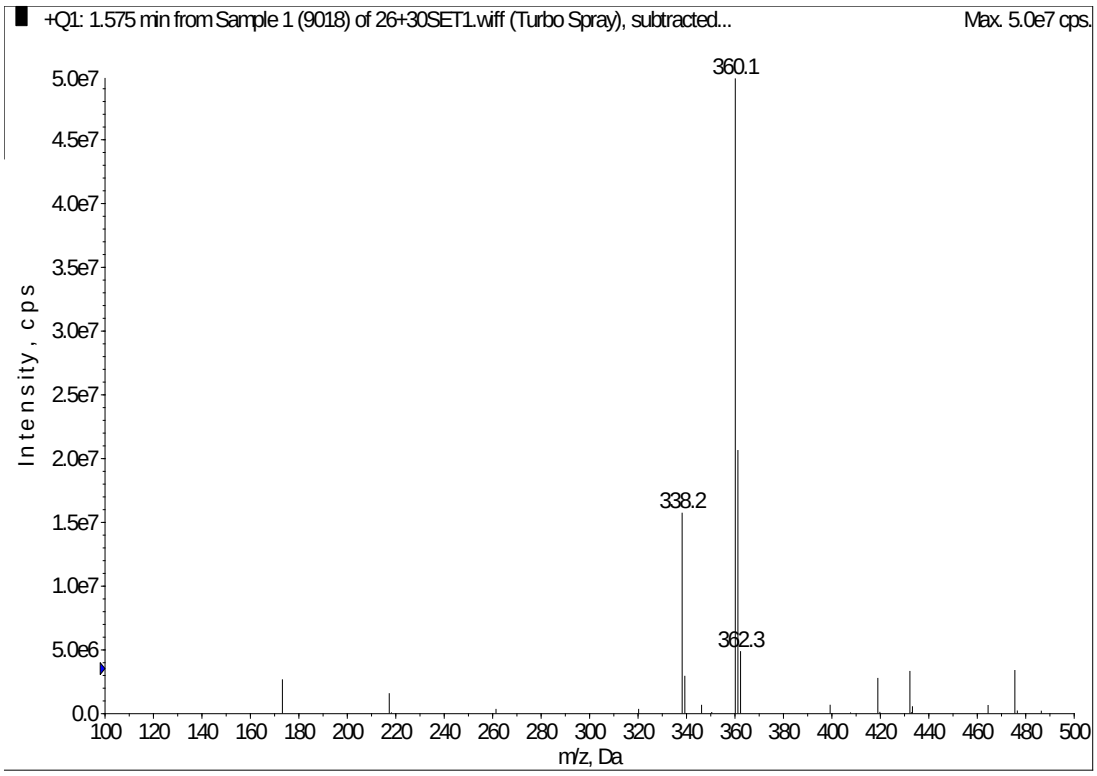


MS of compound **5daa**



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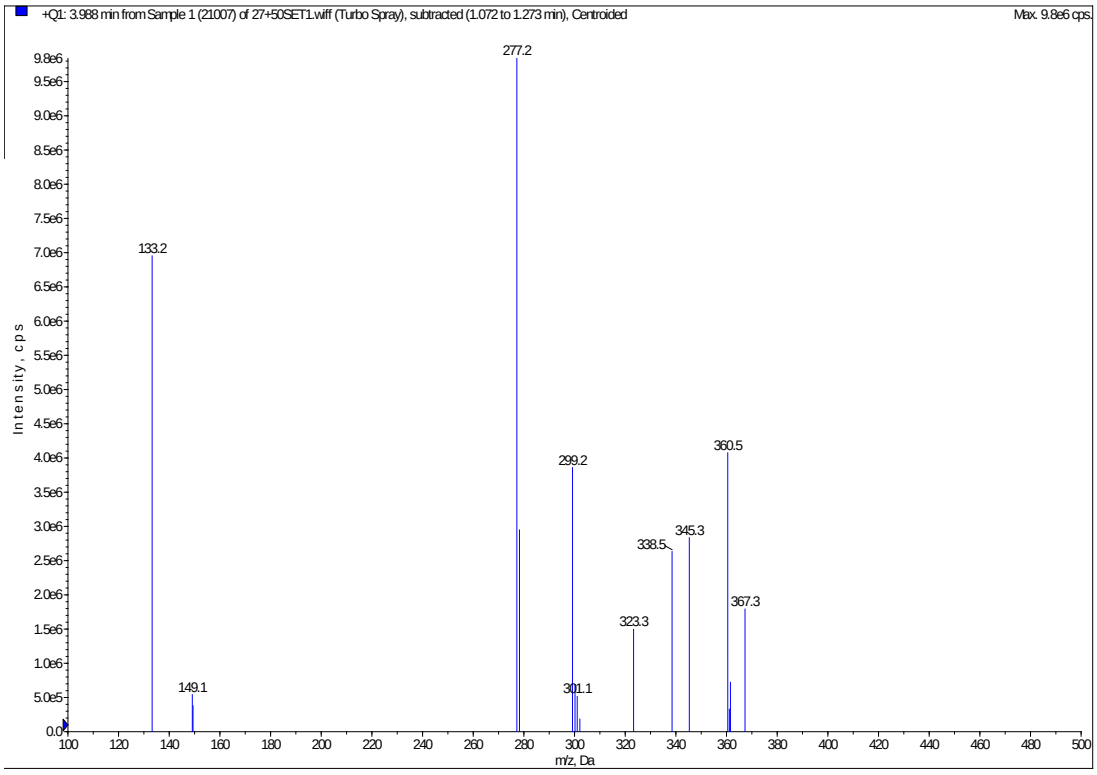
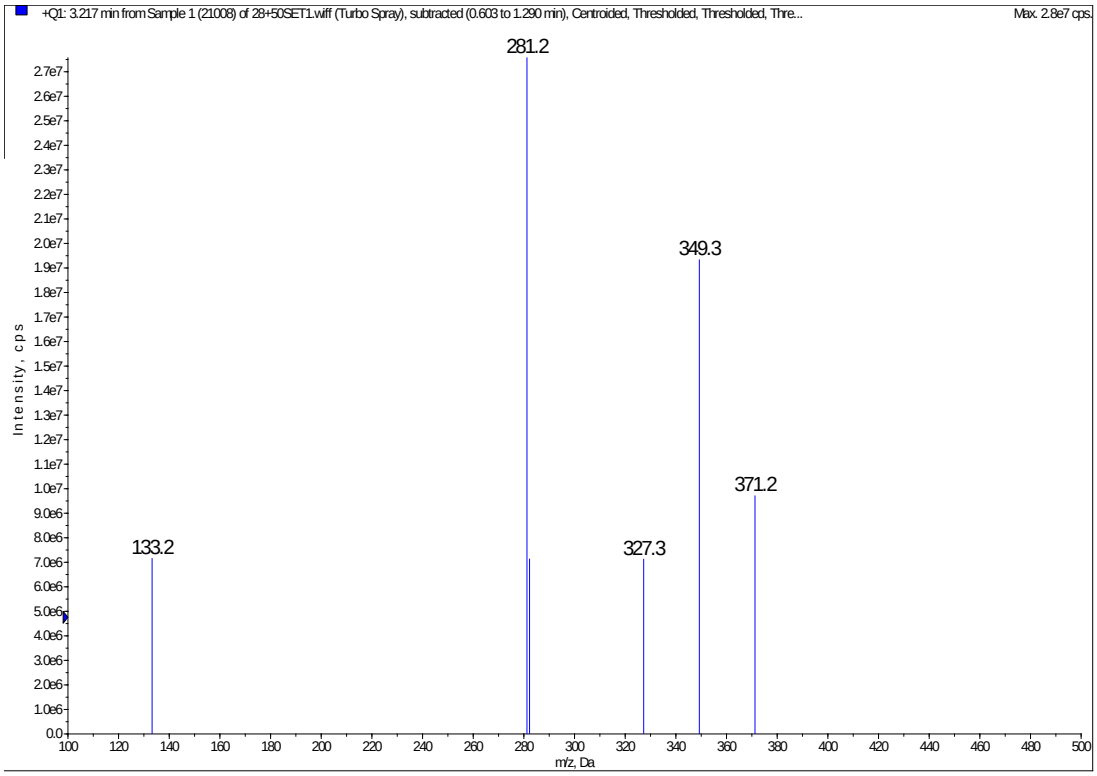
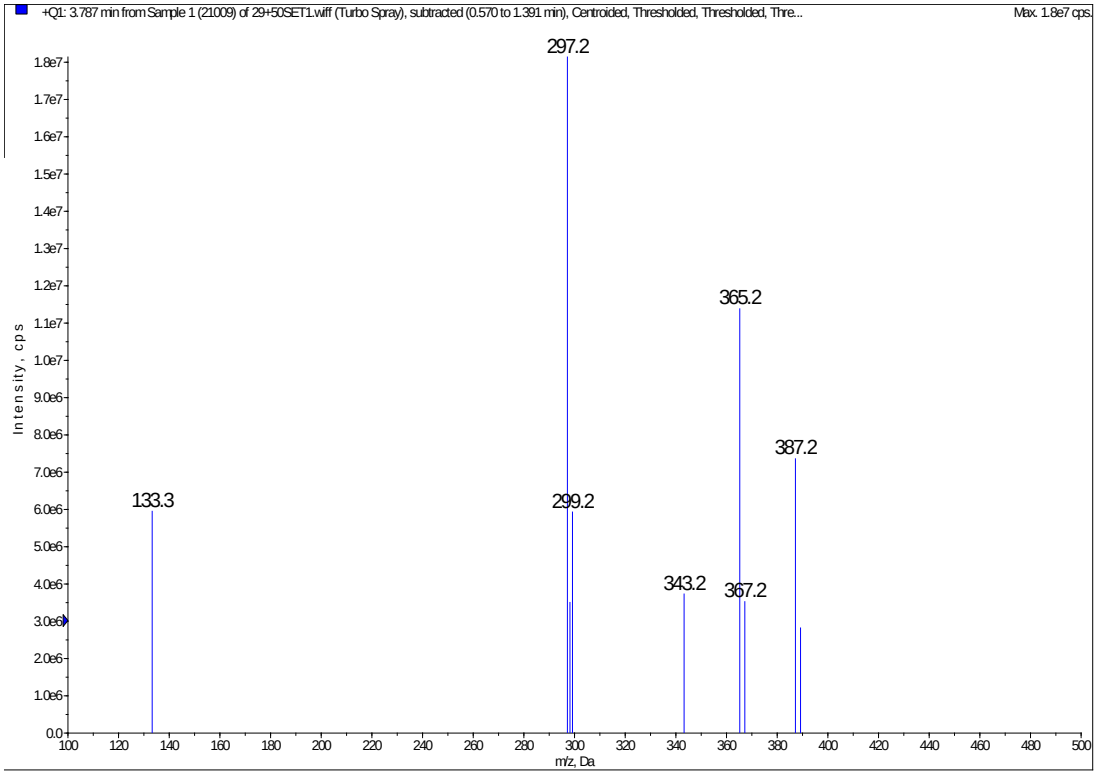


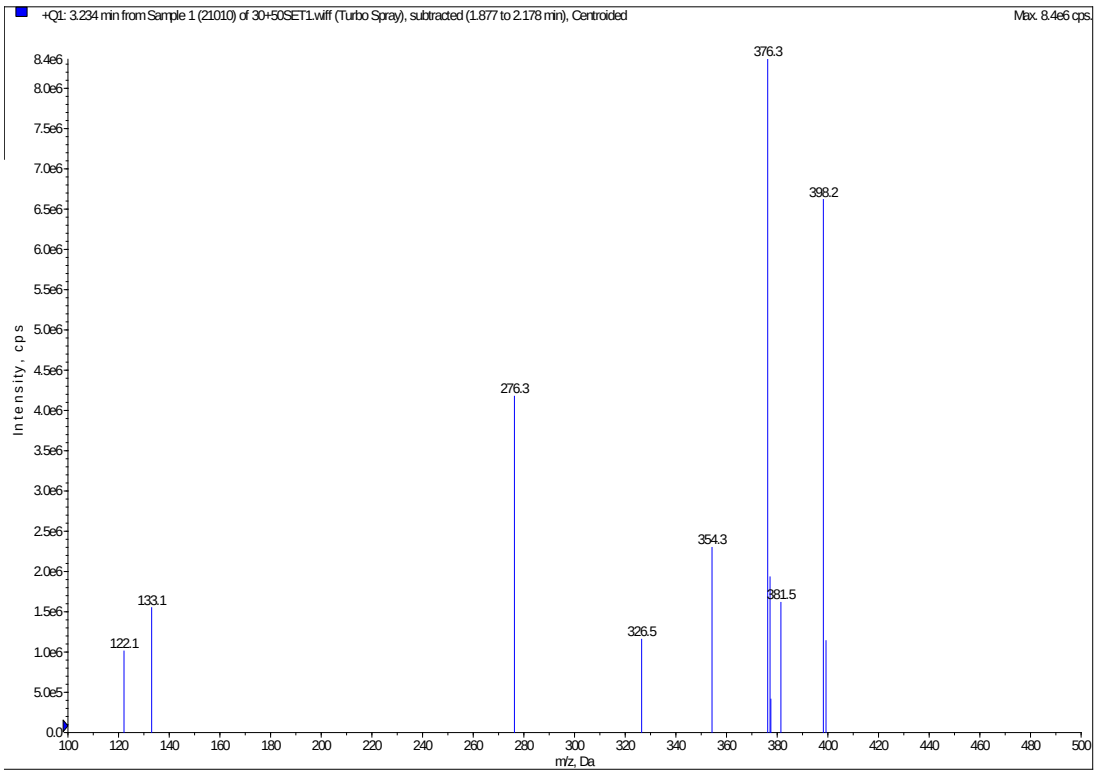
MS of compound **5bbb**



MS of compound **5cbb**



MS of compound **5dbb**



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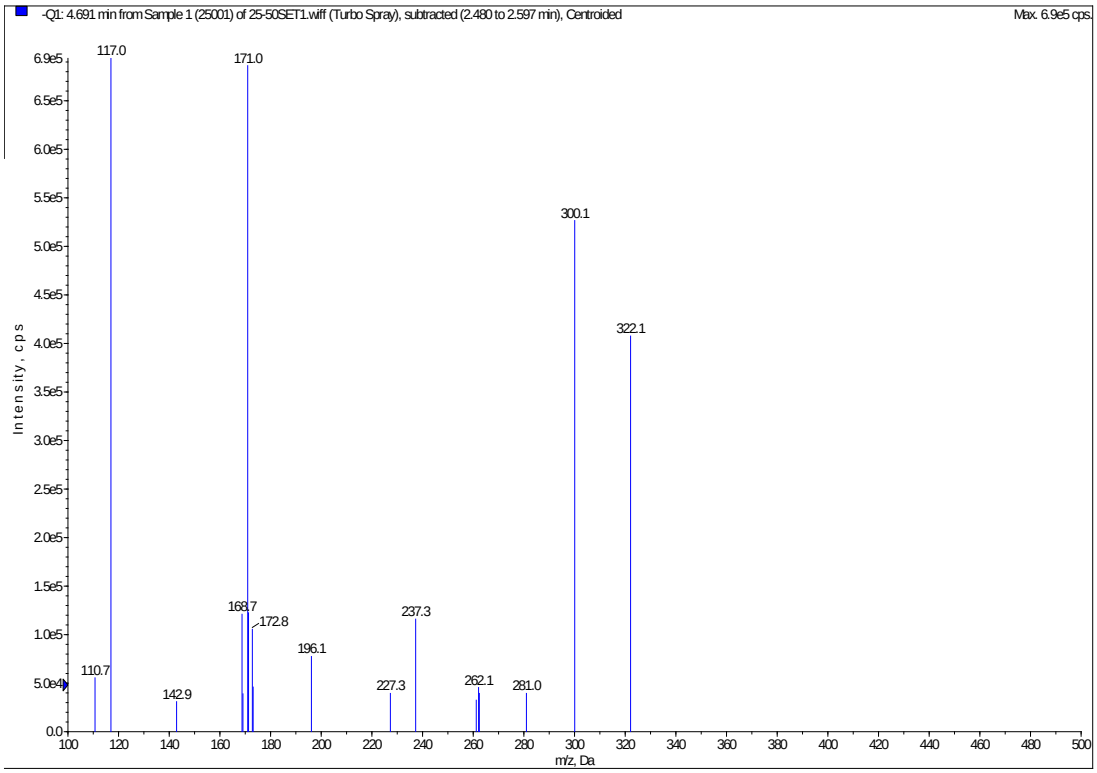
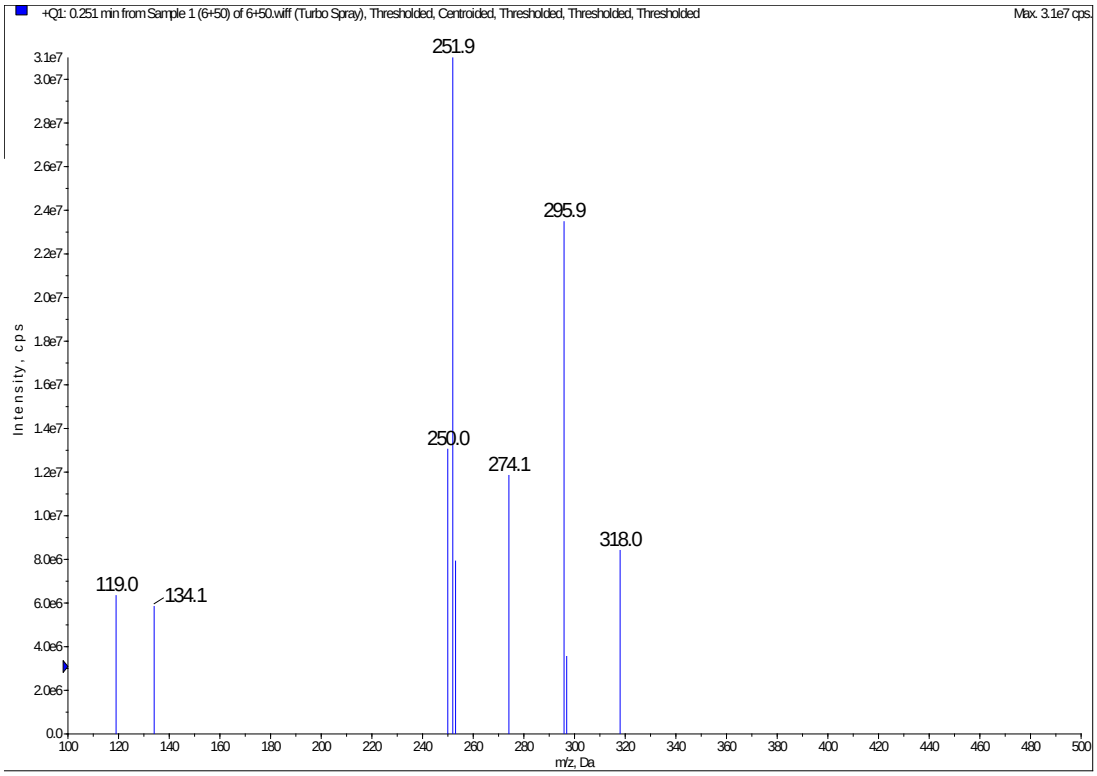
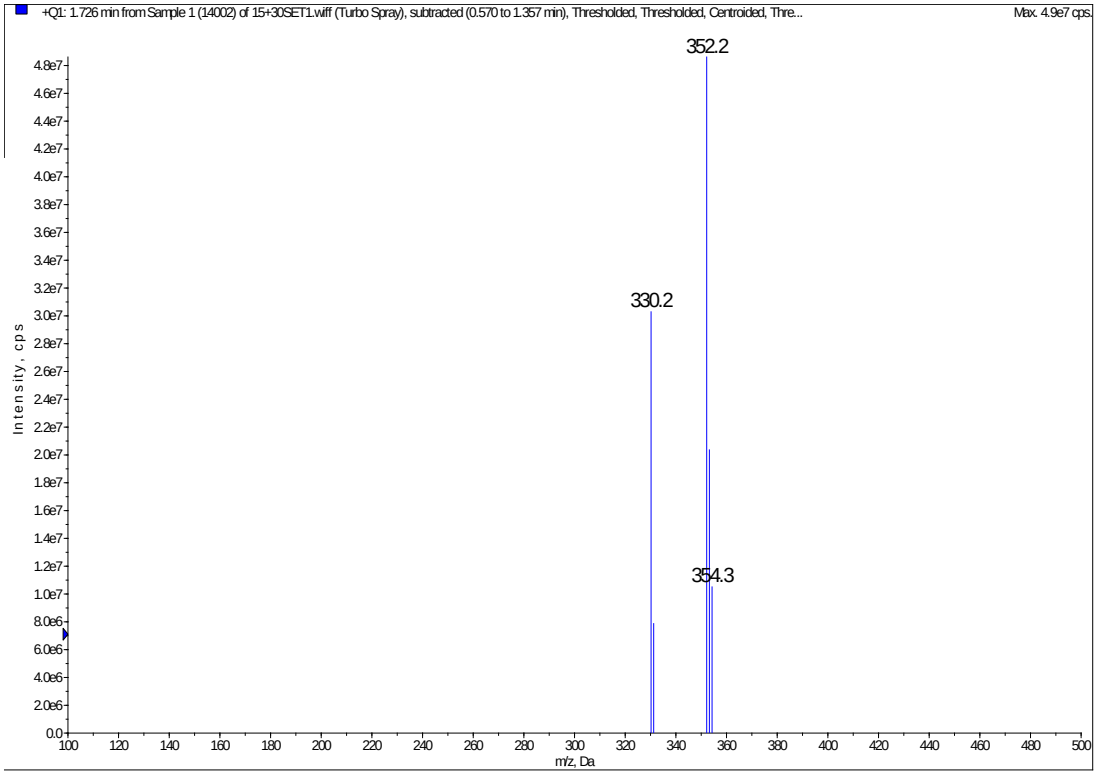


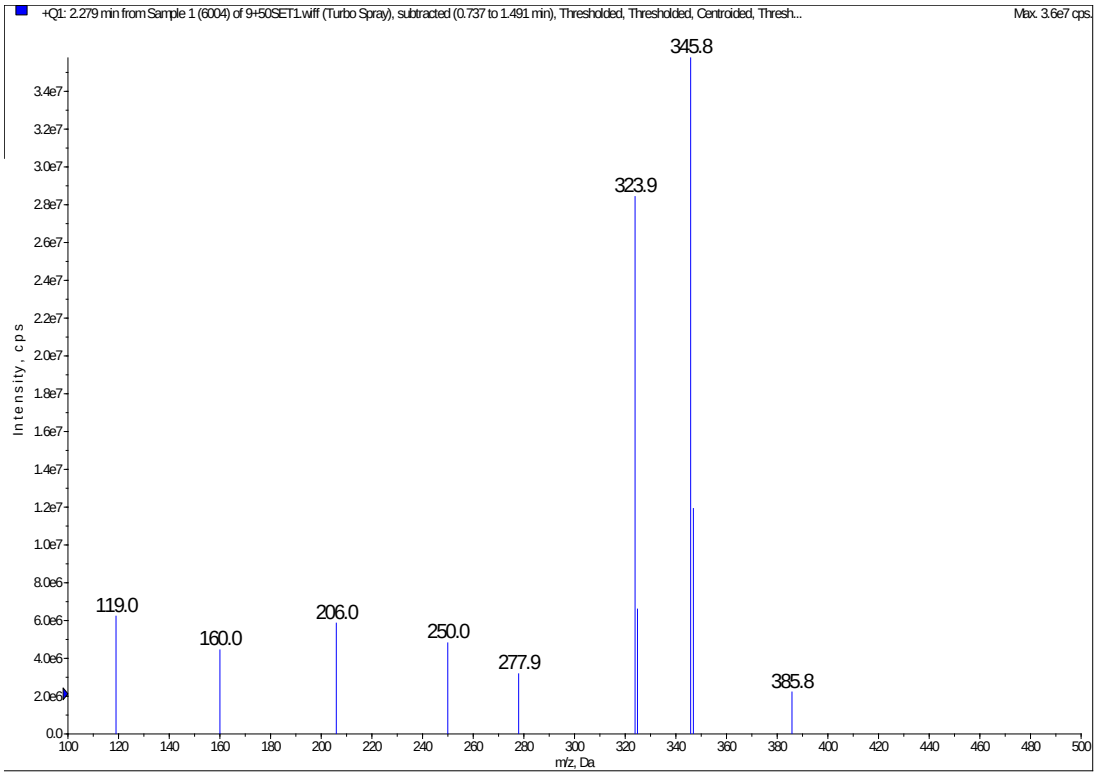
MS of compound **5fab**



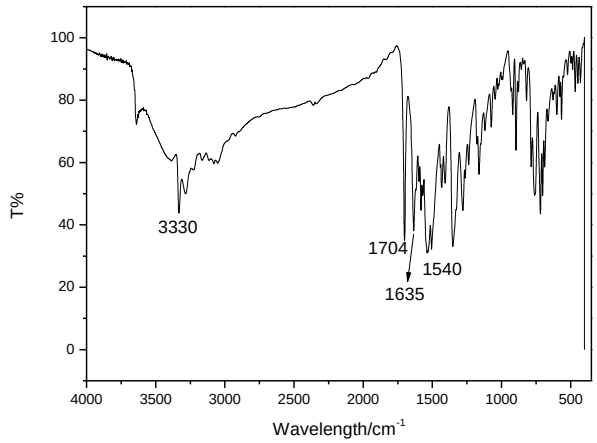
MS of compound **5gab**



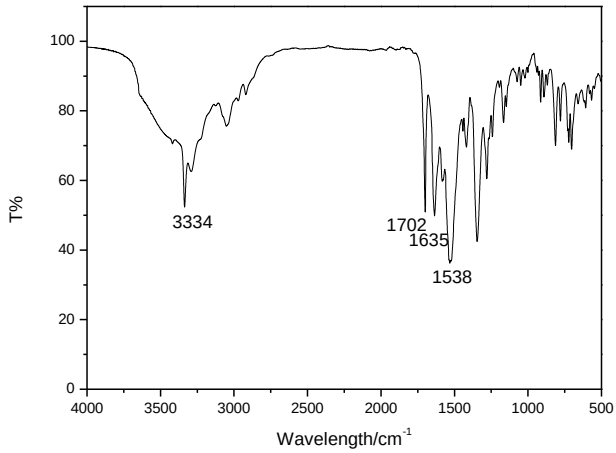
MS of compound **5fac**



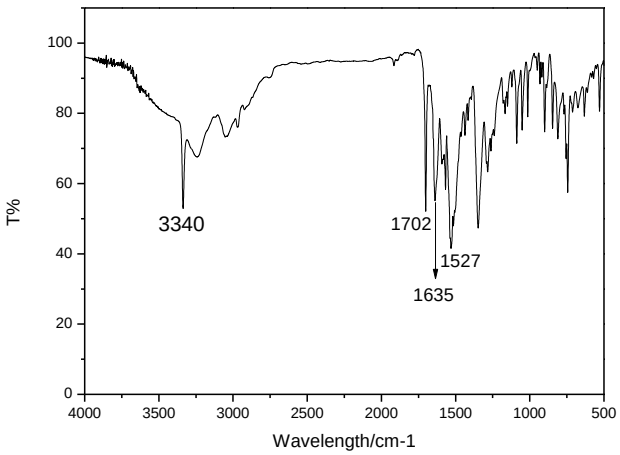
MS of compound **5gac**



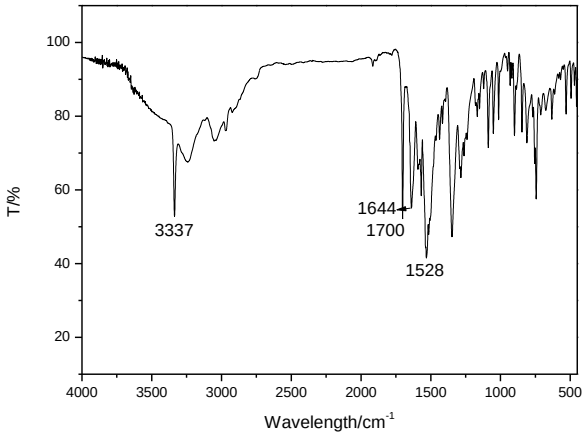
IR spectra of compound **5aaa**



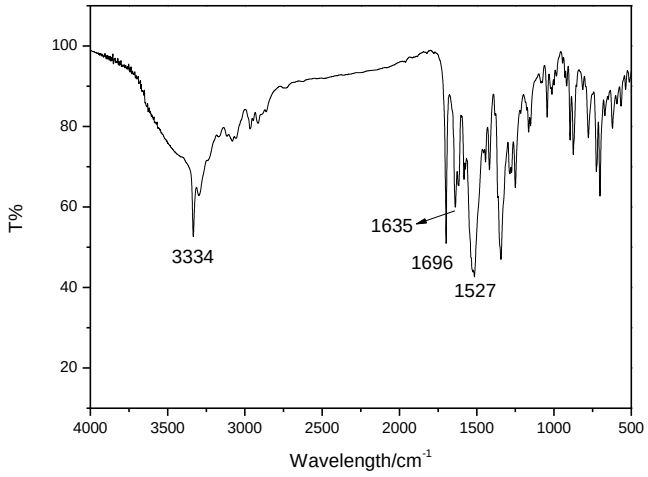
IR spectra of compound **5aba**



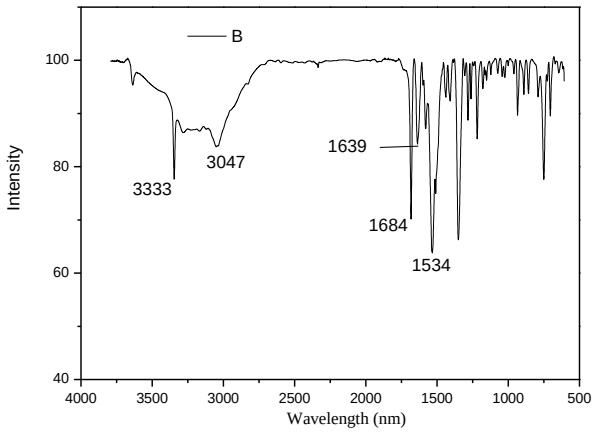
IR spectra of compound **5aca**



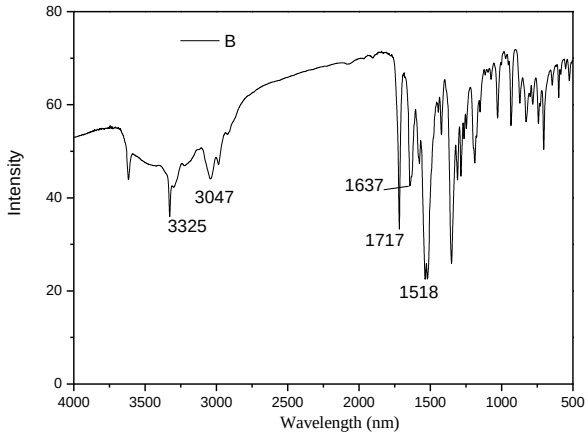
IR spectra of compound **5ada**



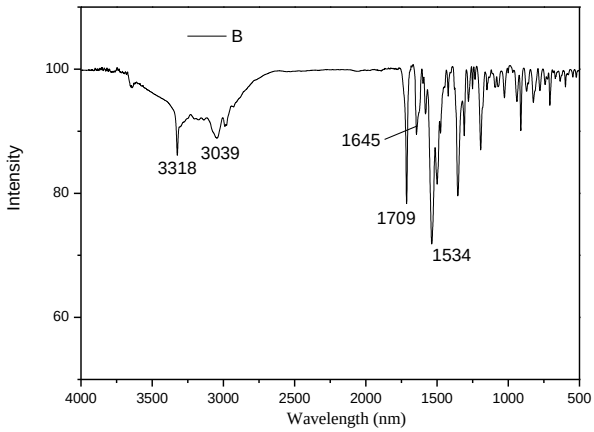
IR spectra of compound **5aea**



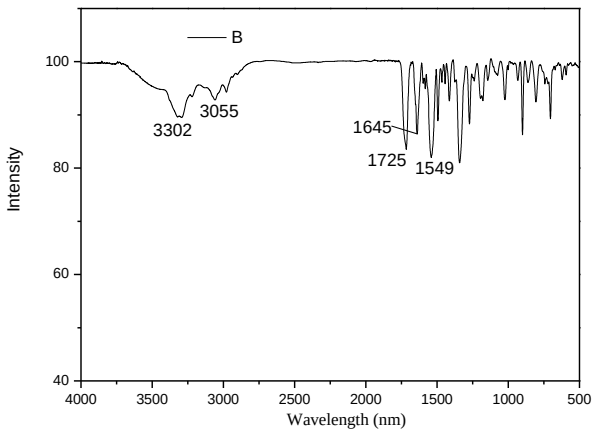
IR spectra of compound **5aab**



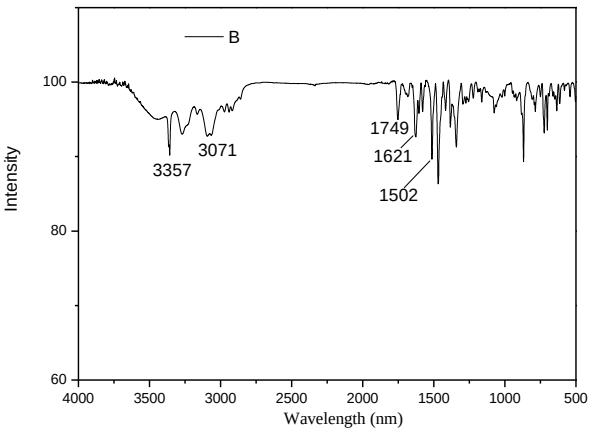
IR spectra of compound **5abb**



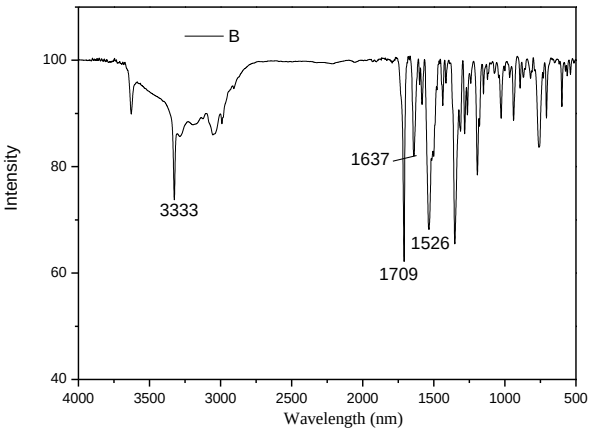
IR spectra of compound **5acb**



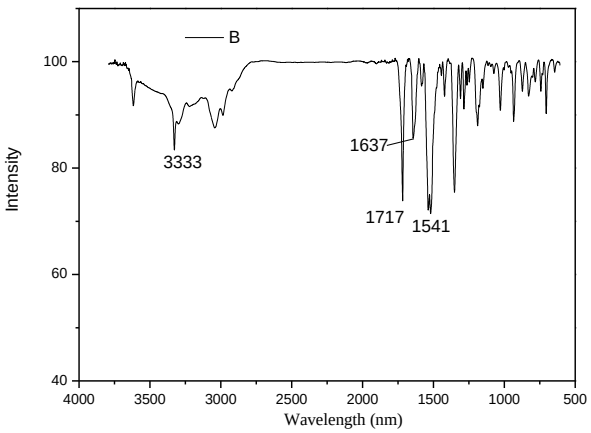
IR spectra of compound **5adb**



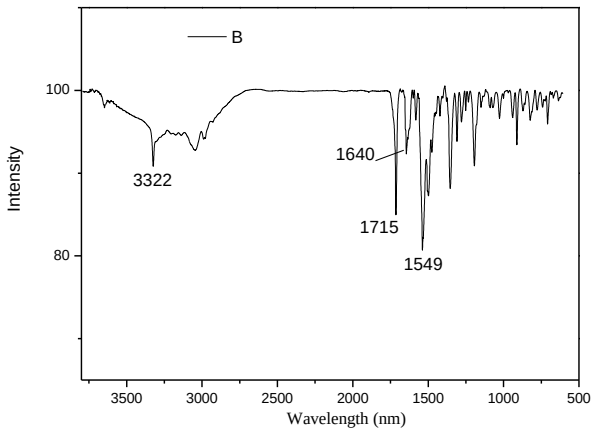
IR spectra of compound **5aeb**



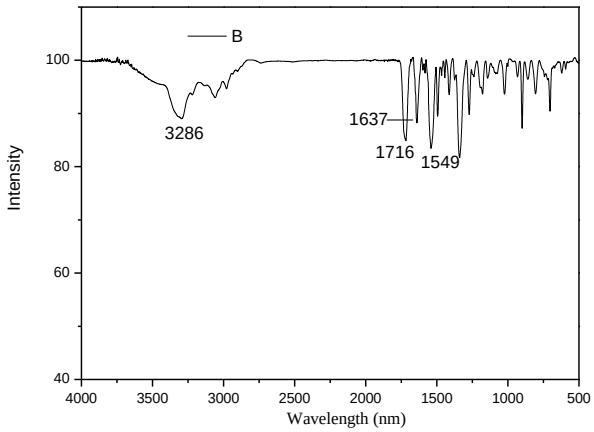
IR spectra of compound **5aac**



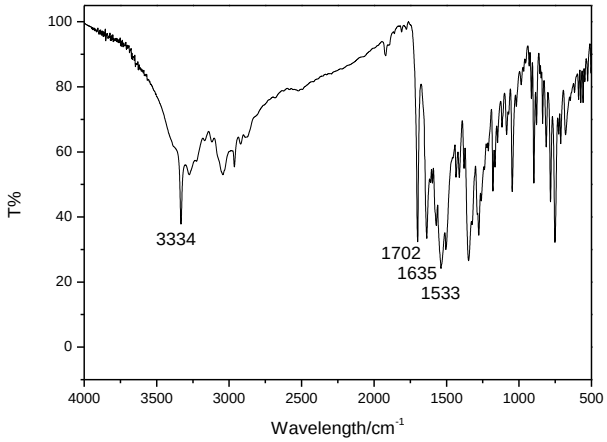
IR spectra of compound **5abc**



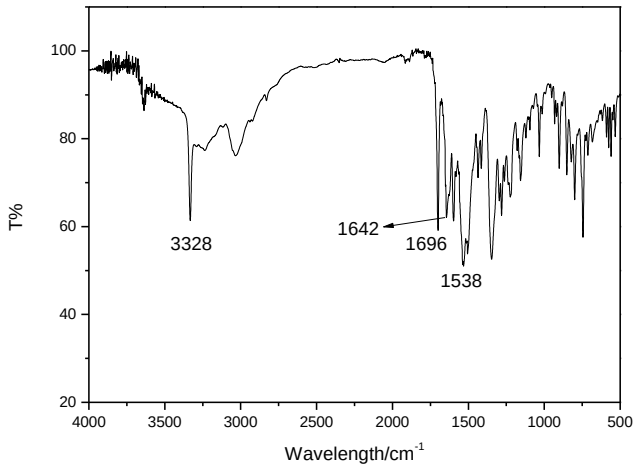
IR spectra of compound **5acc**



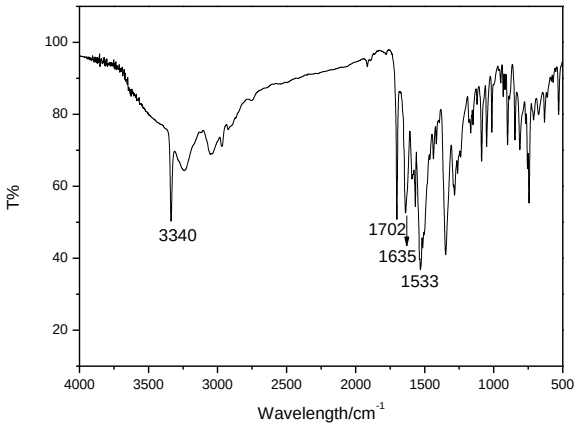
IR spectra of compound **5adc**



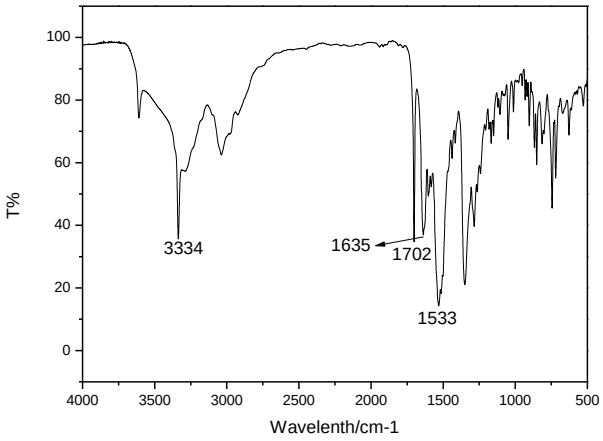
IR spectra of compound **5baa**



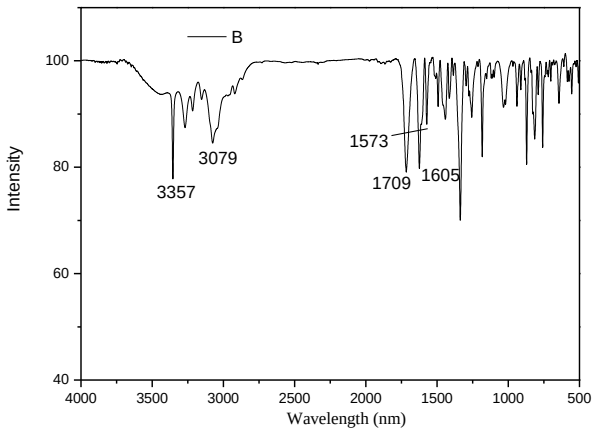
IR spectra of compound **5caa**



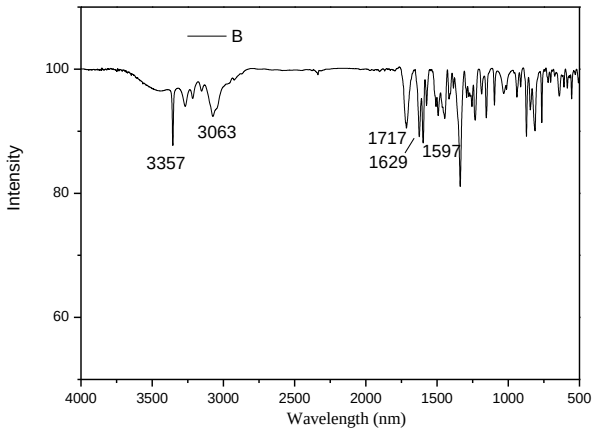
IR spectra of compound **5daa**



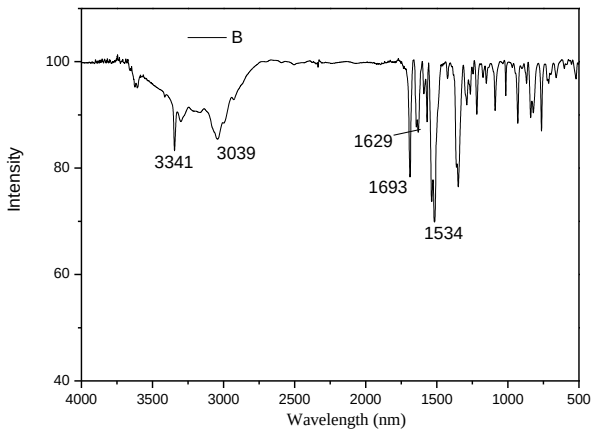
IR spectra of compound **5eaa**



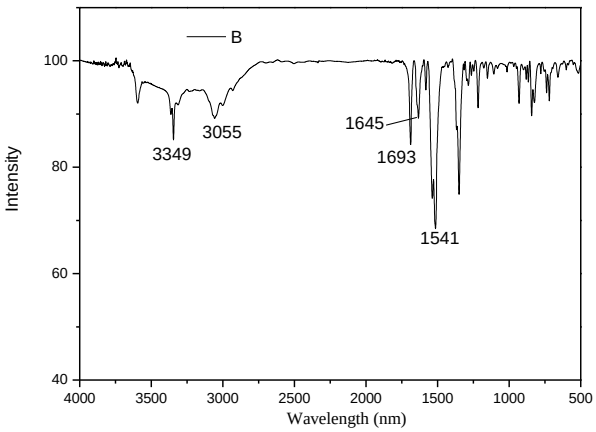
IR spectra of compound **5bbb**



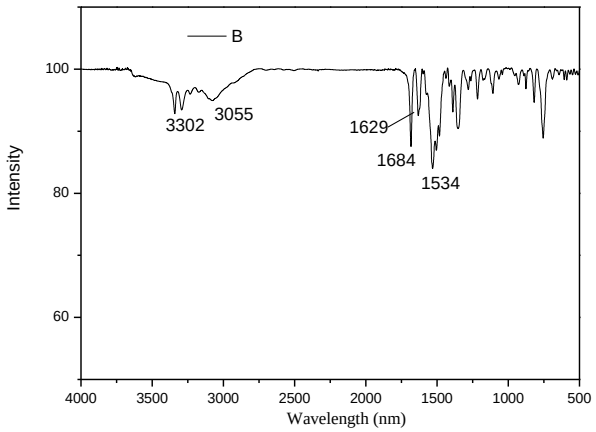
IR spectra of compound **5cbb**



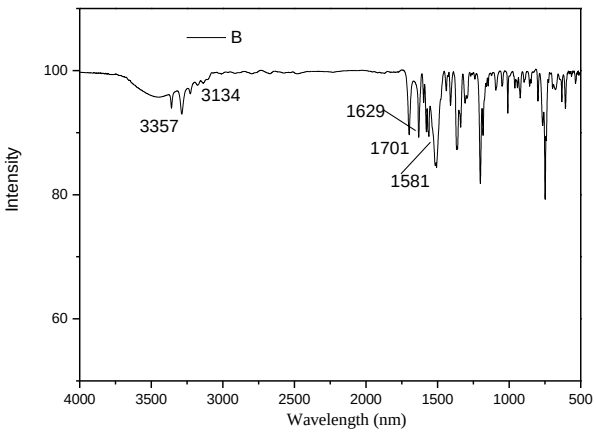
IR spectra of compound **5dbb**



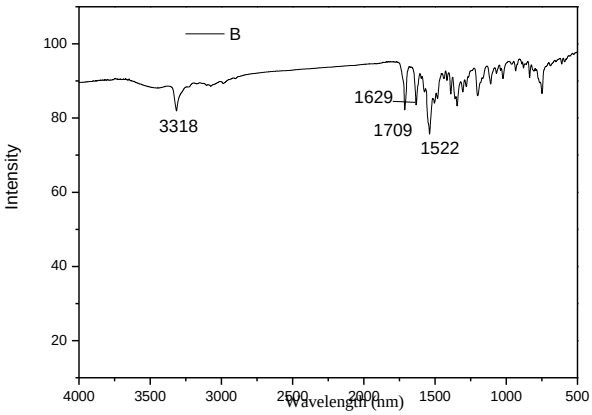
IR spectra of compound **5ebb**



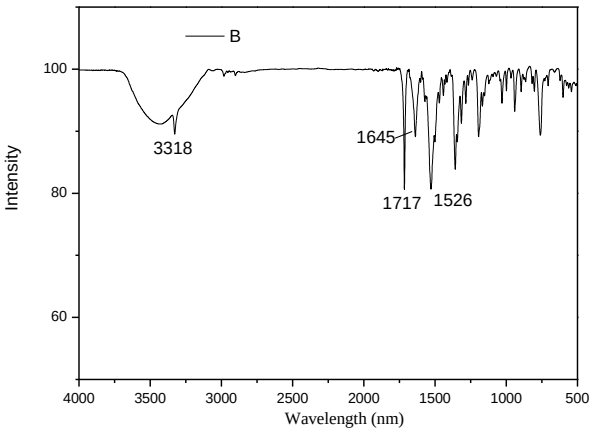
IR spectra of compound **5fab**



IR spectra of compound **5gab**



IR spectra of compound **5fac**



IR spectra of compound **5gac**